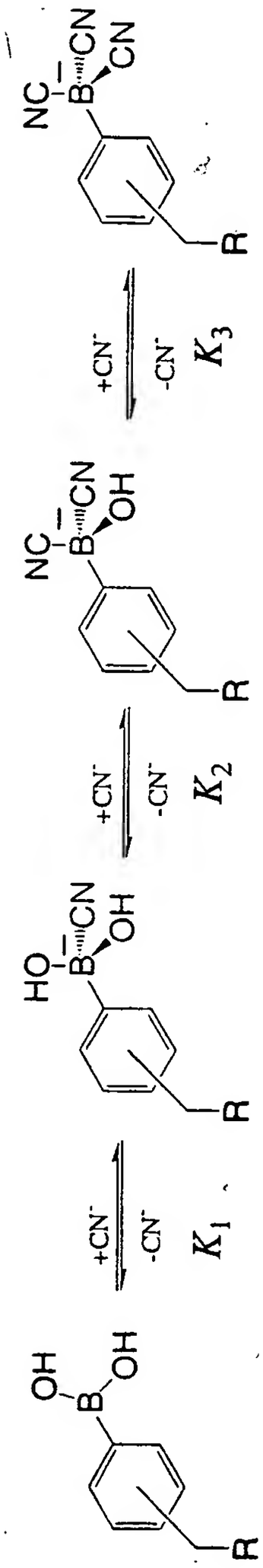
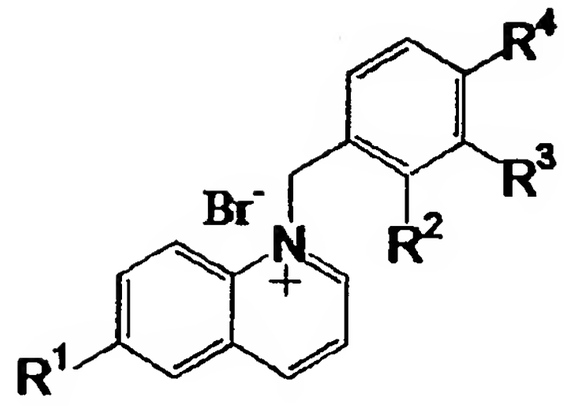


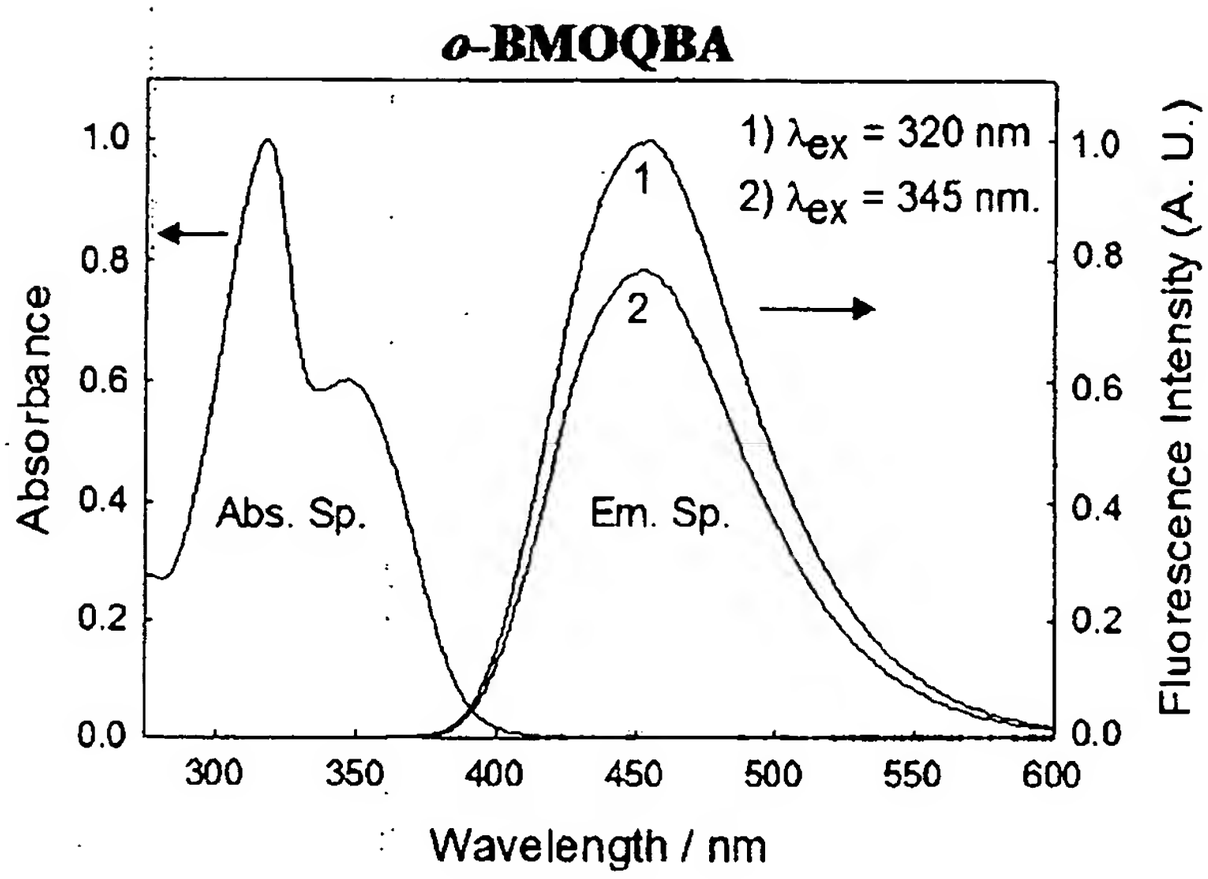
FIGURE 1



Probe	R^1	R^2	R^3	R^4
***o*-BMOQBA**	OCH_3	$B(OH)_2$	H	H
***m*-BMOQBA**	OCH_3	H	$B(OH)_2$	H
***p*-BMOQBA**	OCH_3	H	H	$B(OH)_2$
BMOQ	OCH_3	H	H	H
***o*-BMQBA**	CH_3	$B(OH)_2$	H	H
***m*-BMQBA**	CH_3	H	$B(OH)_2$	H
***p*-BMQBA**	CH_3	H	H	$B(OH)_2$
BMQ	CH_3	H	H	H

FIGURE 2

A


o-BMOQBA
1) λex = 320 nm
2) λex = 345 nm.
1
2
Abs. Sp.
Em. Sp.
Absorbance
Fluorescence Intensity (A. U.)
1.0
0.8
0.6
0.4
0.2
0.0
300
350
400
450
500
550
600
Wavelength / nm

B

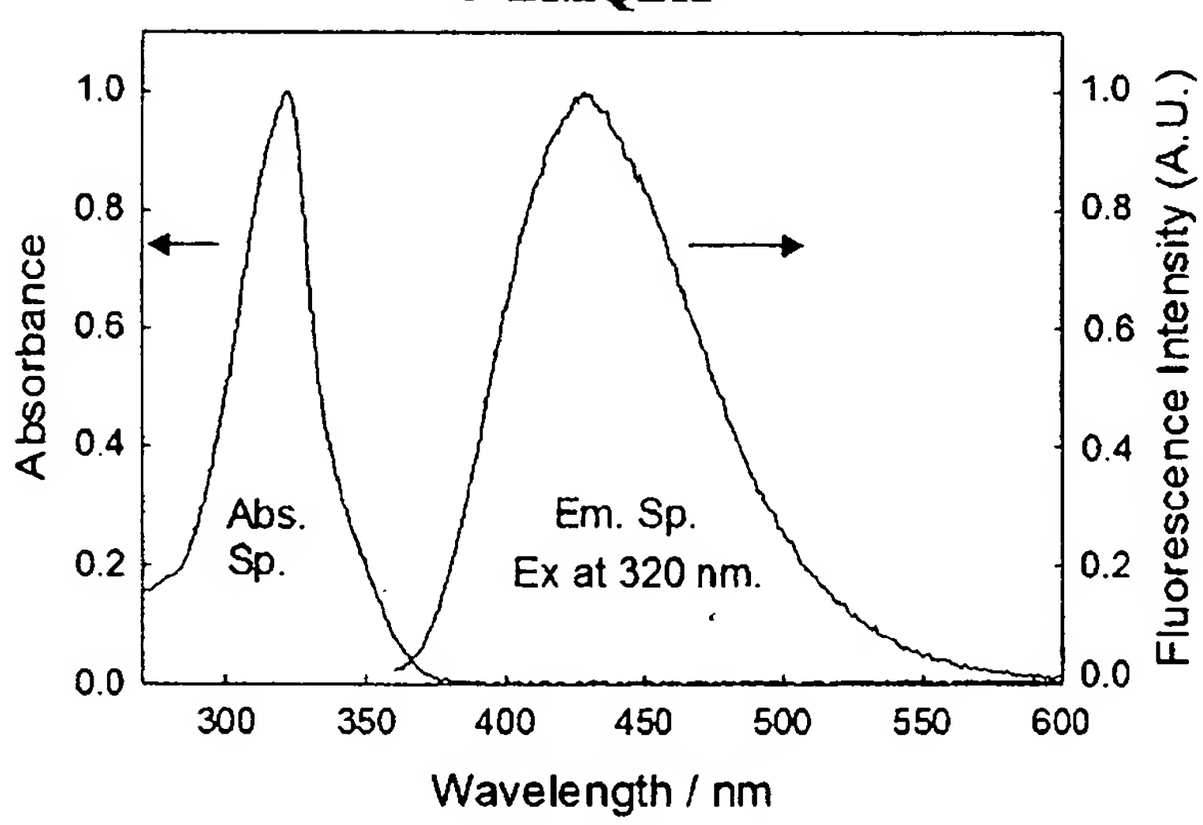
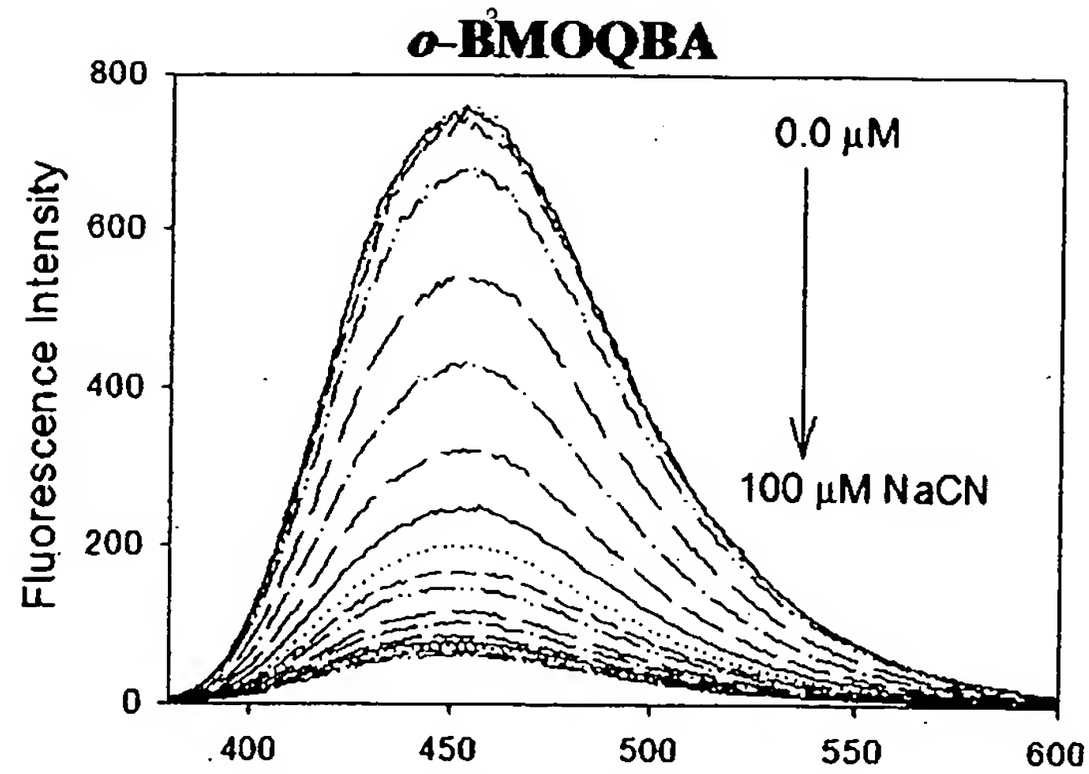
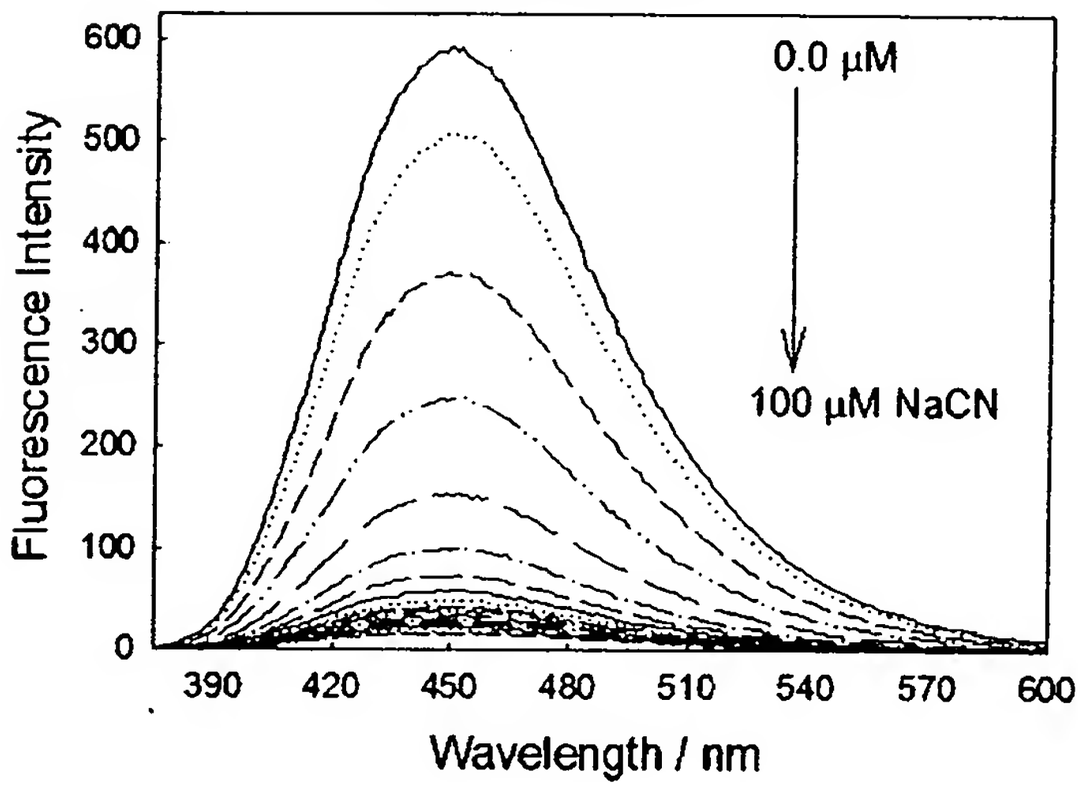

o-BMOQBA
Abs.
Sp.
Em. Sp.
Ex at 320 nm.
Absorbance
Fluorescence Intensity (A.U.)
1.0
0.8
0.6
0.4
0.2
0.0
300
350
400
450
500
550
600
Wavelength / nm

FIGURE 3

A


o-BMOQBA
Fluorescence Intensity
800
600
400
200
0
0.0 µM
100 µM NaCN
400
450
500
550
600
Wavelength / nm

B


m-BMOQBA
Fluorescence Intensity
600
500
400
300
200
100
0
0.0 µM
100 µM NaCN
390
420
450
480
510
540
570
600
Wavelength / nm

C

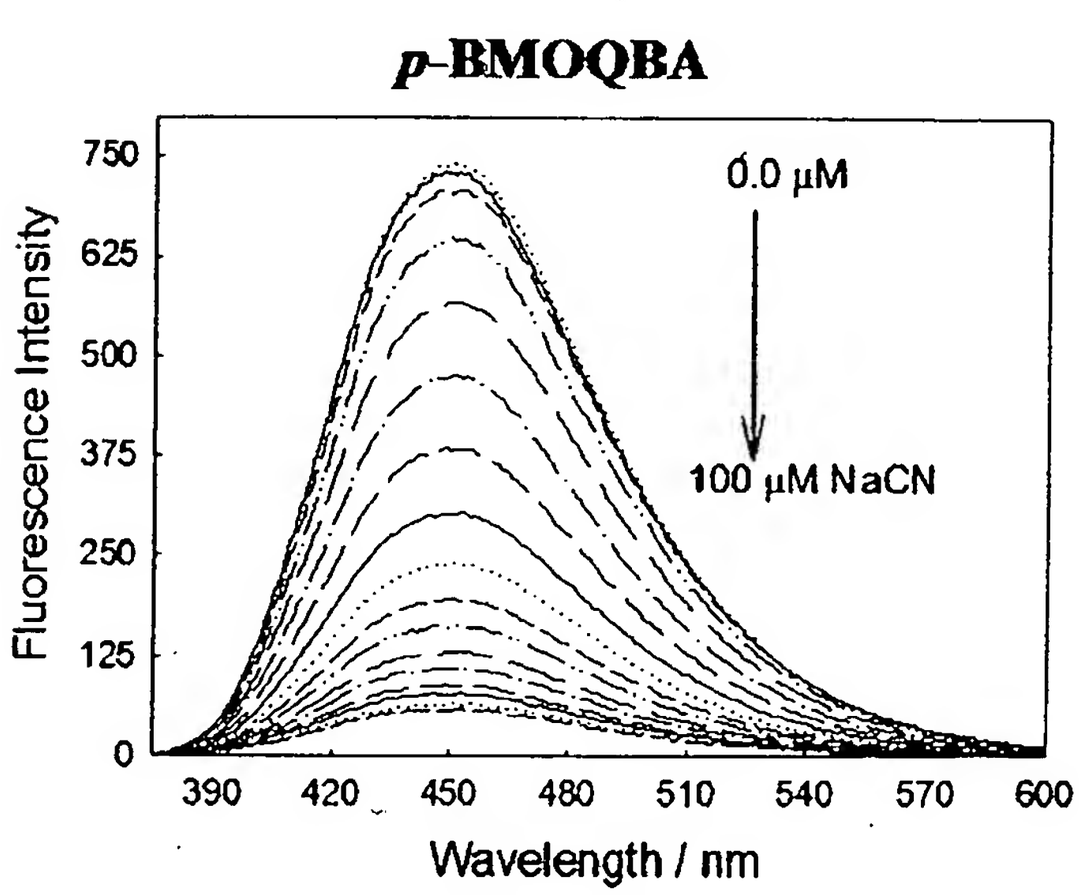

p-BMOQBA
Fluorescence Intensity
750
625
500
375
250
125
0
0.0 µM
100 µM NaCN
390
420
450
480
510
540
570
600
Wavelength / nm

FIGURE 4

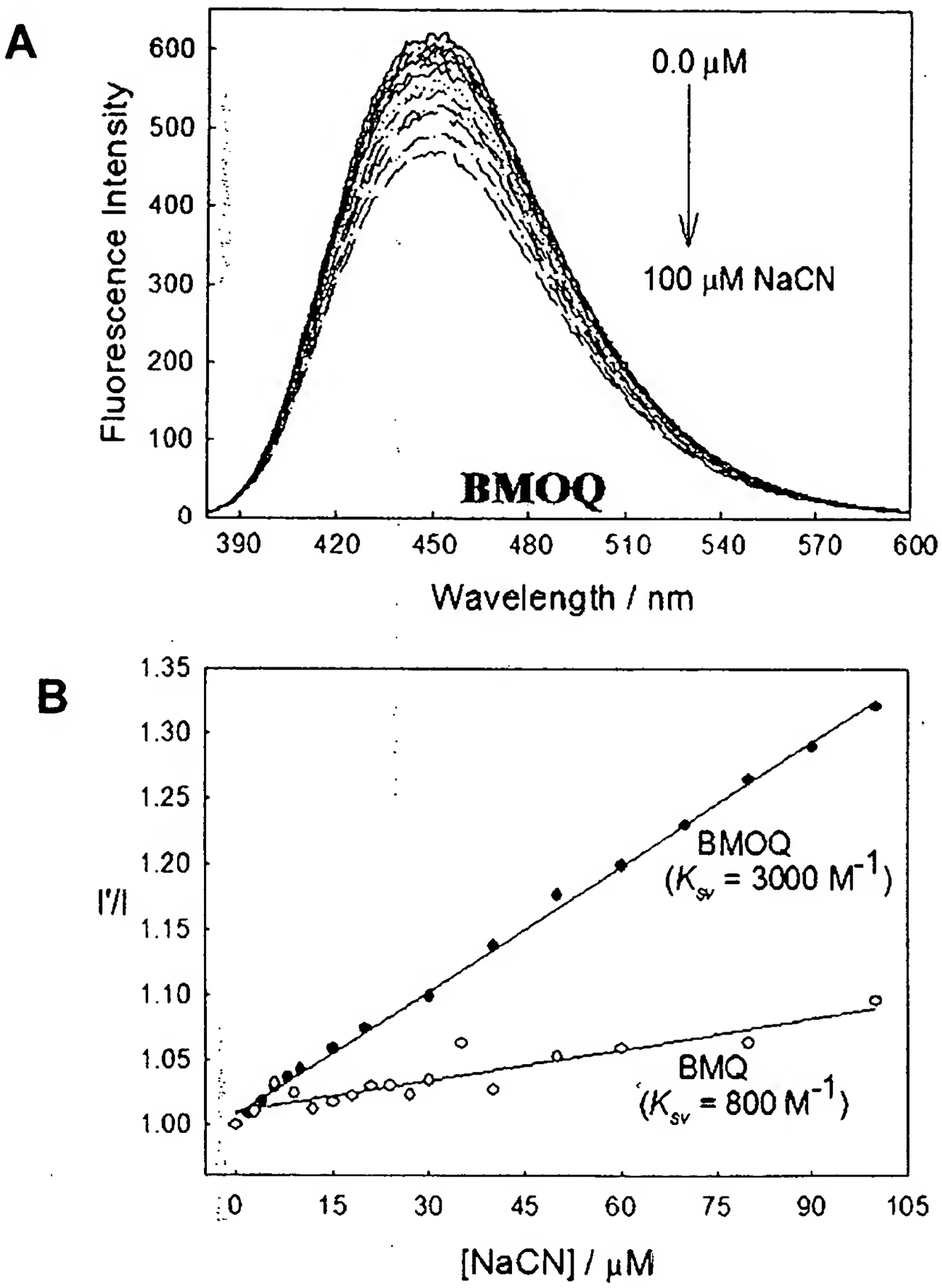

A
Fluorescence Intensity
600
500
400
300
200
100
0
0.0 µM
100 µM NaCN
BMOQ
390
420
450
480
510
540
570
600
Wavelength / nm
B
I'/I
1.35
1.30
1.25
1.20
1.15
1.10
1.05
1.00
BMOQ
(K_{sv} = 3000 M^{-1})
BMQ
(K_{sv} = 800 M^{-1})
0
15
30
45
60
75
90
105
[NaCN] / µM

FIGURE 5

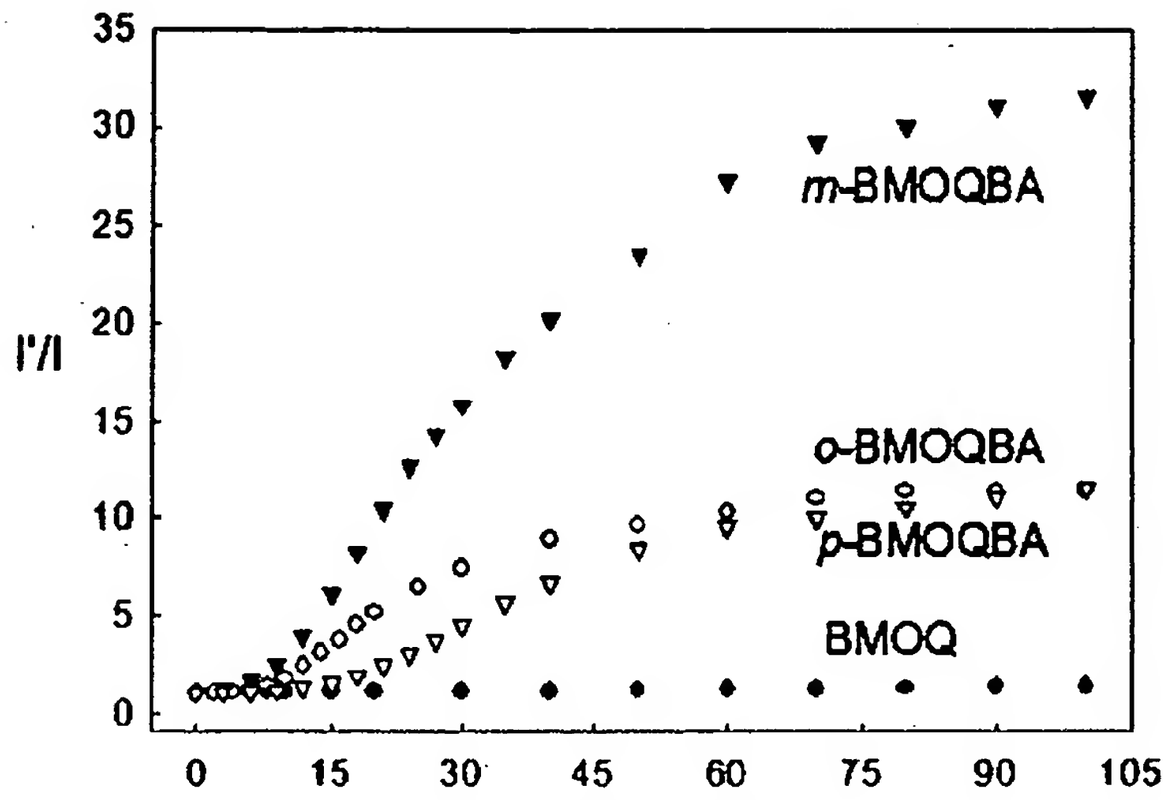

35
30
25
20
15
10
5
0
I'/I
0
15
30
45
60
75
90
105
[NaCN] / μM
m-BMOQBA
o-BMOQBA
p-BMOQBA
BMOQ

FIGURE 6

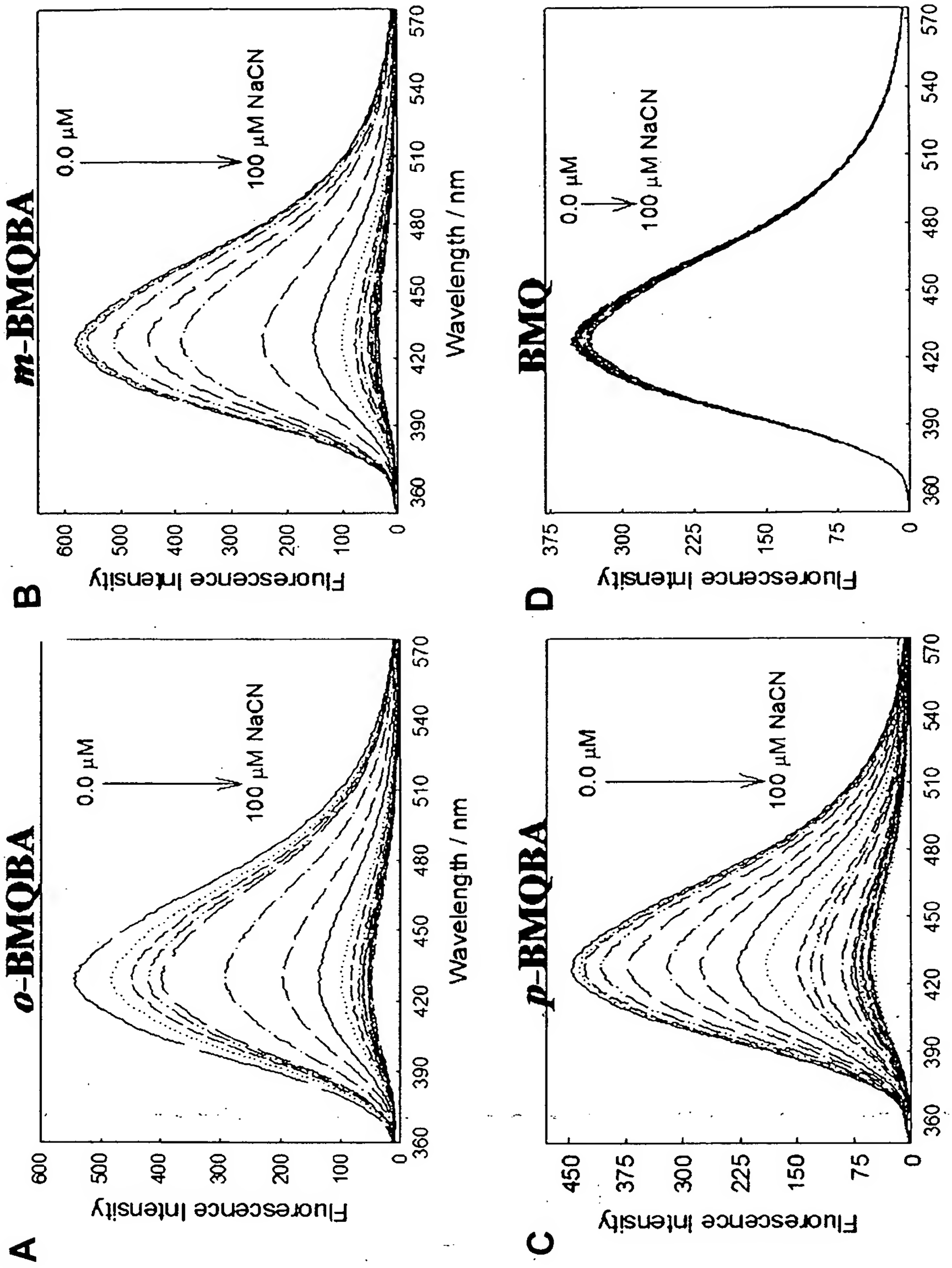

m-BMQBA
BMQ
o-BMQBA
p-BMQBA
0.0 µM
100 µM NaCN
Wavelength / nm
Fluorescence Intensity
A
B
C
D

FIGURE 7

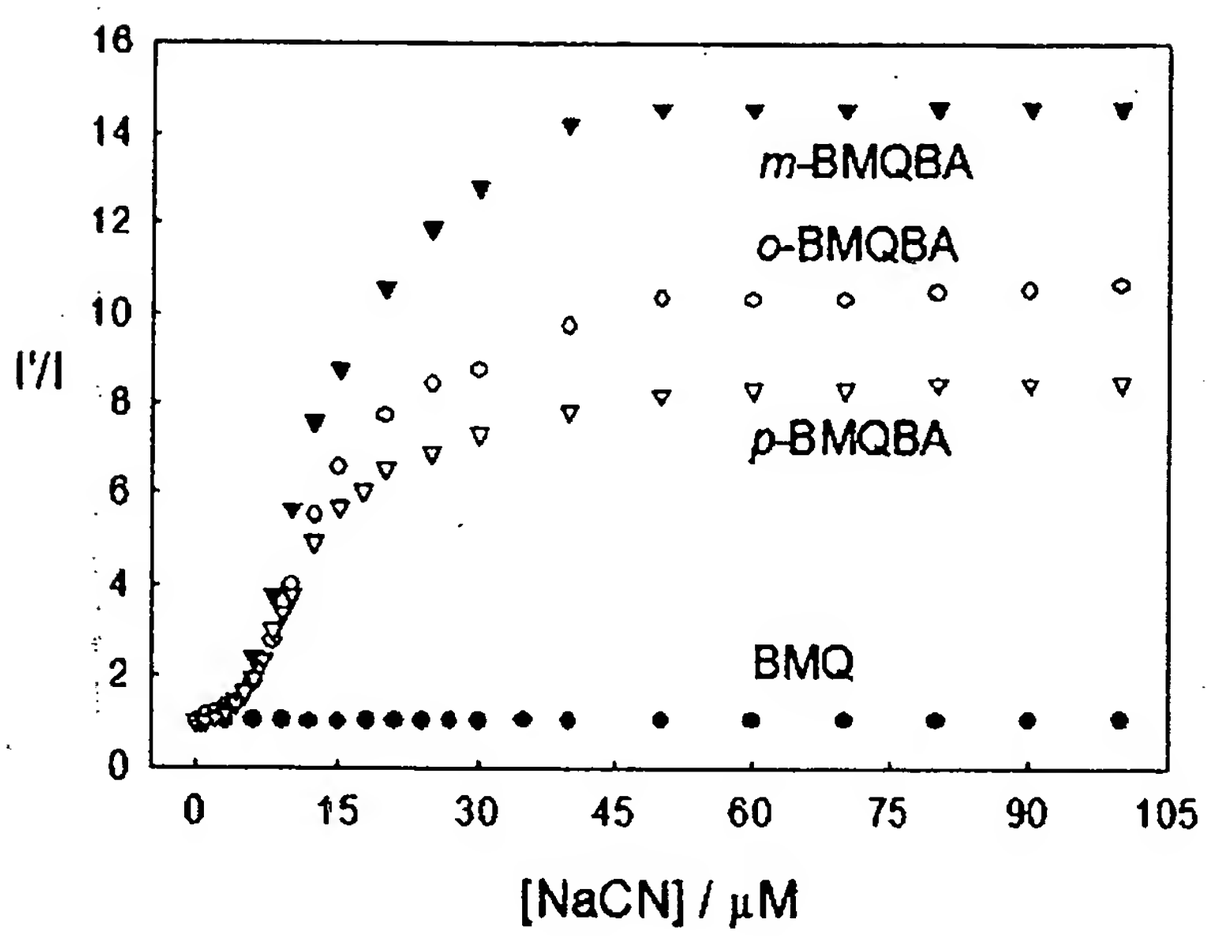

16
14
12
10
8
6
4
2
0
I'/I
0
15
30
45
60
75
90
105
[NaCN] / µM
m-BMQBA
o-BMQBA
p-BMQBA
BMQ

FIGURE 8

Table 1 - Dissociation constants, K_D (μM^3), for the probes with cyanide in water.

Probe	K_D (μM^3)
o-BMOQBA	52.9
m-BMOQBA	84.0
p-BMOQBA	20.8
BMOQ	---
o-BMQBA	16.7
m-BMQBA	16.9
p-BMQBA	15.9
BMQ	---

FIGURE 9

Table 2 – Multiexponential Intensity decay of BMOQ and *o*-BMOQBA

[Cyanide] μM	τ_1 (ns)	α_1	τ_2 (ns)	α_2	$\bar{\tau}$ (ns)	$\langle\tau\rangle$ (ns)	χ^2
*o-BMOQBA							
0	26.71	1.0			26.71	26.71	1.33
5	26.33	1.0			26.33	26.33	1.13
10	26.34	1.0			26.34	26.34	1.21
15	26.19	1.0			26.19	26.19	1.30
25	24.78	1.0			24.78	24.78	1.23
35	0.324	0.0160	25.54	0.9840	25.53	25.14	1.35
45	0.326	0.0184	25.10	0.9816	25.09	24.64	1.46
50	0.455	0.0176	25.20	0.9824	25.19	24.76	1.41
*BMOQ							
0	27.30	1.0			27.30	27.30	1.08
5	27.04	1.0			27.04	27.04	1.10
10	26.74	1.0			26.74	26.74	1.12
15	26.53	1.0			26.53	26.53	1.06
20	26.25	1.0			26.25	26.25	1.14
30	25.86	1.0			25.86	25.86	1.17
40	25.37	1.0			25.37	25.37	1.05
50	25.00	1.0			25.00	25.00	1.16

* λ_{ex} = 372 nm, emission was collected with a 416 nm cut-off filter. BMOQ $K_{SV} \approx 2$ nM^{-1}.

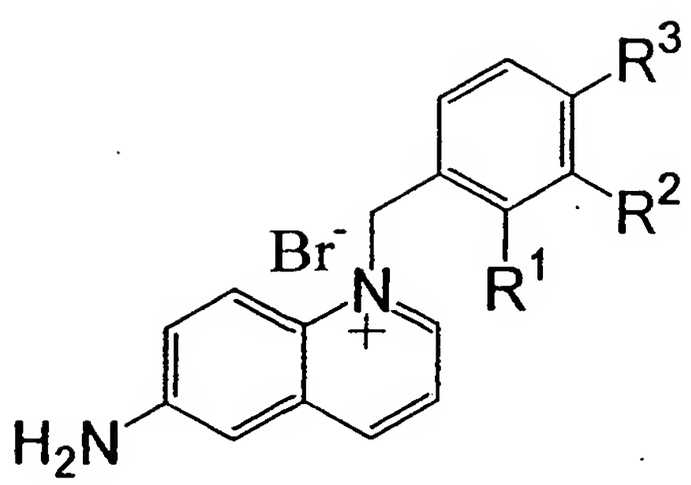
FIGURE 10

Table 3 – Multiexponential Intensity decay of BMQ and *o*-BMQBA

[Cyanide] μM	τ_1 (ns)	α_1	τ_2 (ns)	α_2	$\bar{\tau}$ (ns)	$\langle\tau\rangle$ (ns)	χ^2
***o*-BMQBA**							
0	2.18	0.4646	4.74	0.5354	4.01	3.55	1.00
5	2.14	0.4615	4.45	0.5385	3.78	3.38	1.12
10	2.28	0.5704	4.75	0.4296	3.78	3.34	1.04
15	1.86	0.3265	3.64	0.6735	3.29	3.06	0.97
20	1.88	0.3476	3.69	0.6524	3.30	3.06	1.04
30	1.44	0.1762	3.27	0.8238	3.11	2.95	1.21
40	1.92	0.3511	3.59	0.6489	3.21	3.00	0.90
50	1.87	0.3320	3.58	0.6680	3.22	3.01	1.07
***BMQ**							
0	2.59	1.0			2.59	2.59	1.07
5	2.58	1.0			2.58	2.58	1.09
10	2.59	1.0			2.59	2.59	1.07
15	2.57	1.0			2.57	2.57	1.02
20	2.57	1.0			2.57	2.57	1.12
30	2.55	1.0			2.55	2.55	1.08
40	2.55	1.0			2.55	2.55	1.14
50	2.55	1.0			2.55	2.55	1.17

* λ_{ex} = 372 nm, emission was collected with a 416 nm cut-off filter. BMQ $K_{sv} \approx 0.4$ nM^{-1}.

FIGURE 11



Probe	R^1	R^2	R^3
***o*-BAQBA**	$B(OH)_2$	H	H
***m*-BAQBA**	H	$B(OH)_2$	H
***p*-BAQBA**	H	H	$B(OH)_2$
BAQ	H	H	H

FIGURE 12

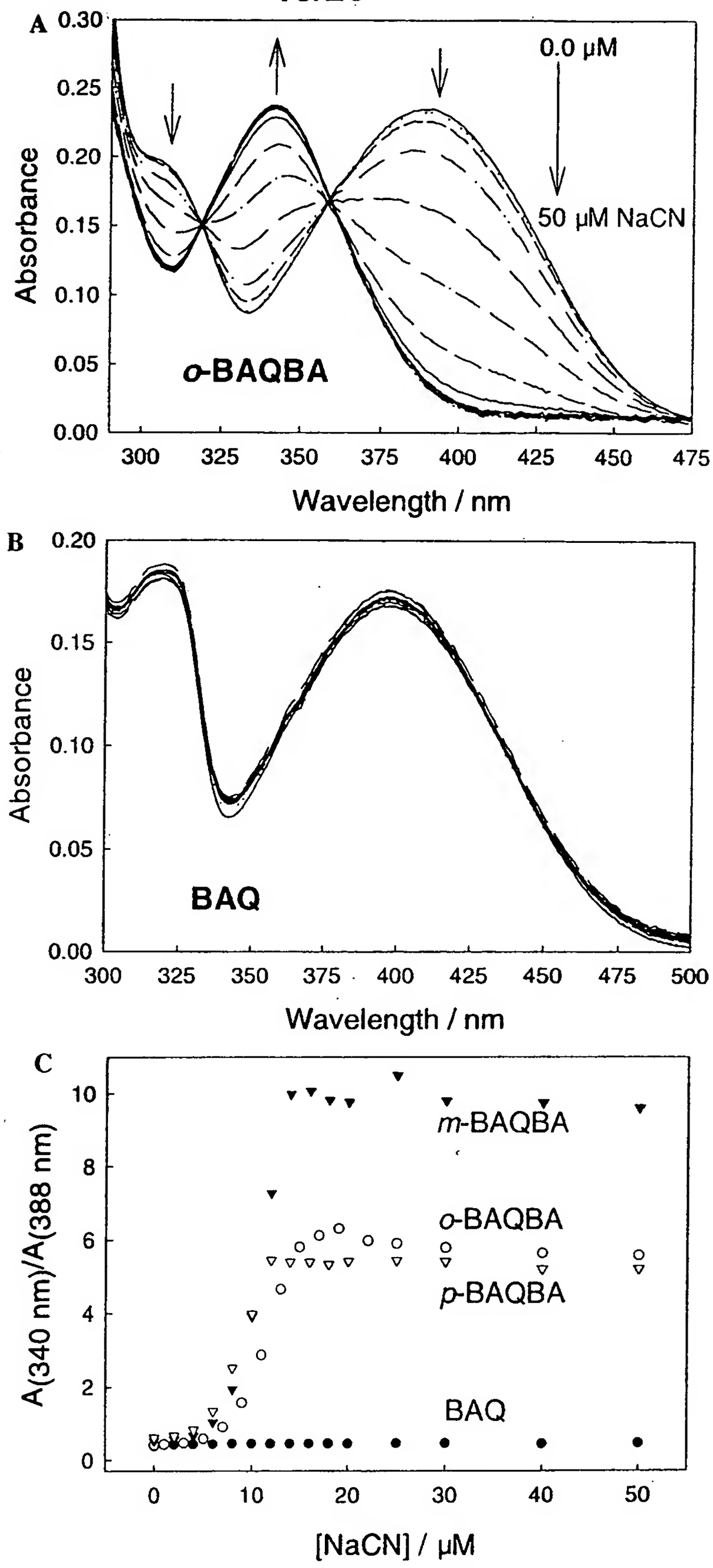

A
Absorbance
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0.0 μM
50 μM NaCN
o-BAQBA
300
325
350
375
400
425
450
475
Wavelength / nm
B
Absorbance
0.20
0.15
0.10
0.05
0.00
BAQ
300
325
350
375
400
425
450
475
500
Wavelength / nm
C
A(340 nm)/A(388 nm)
10
8
6
4
2
0
m-BAQBA
o-BAQBA
p-BAQBA
BAQ
0
10
20
30
40
50
[NaCN] / μM

FIGURE 13

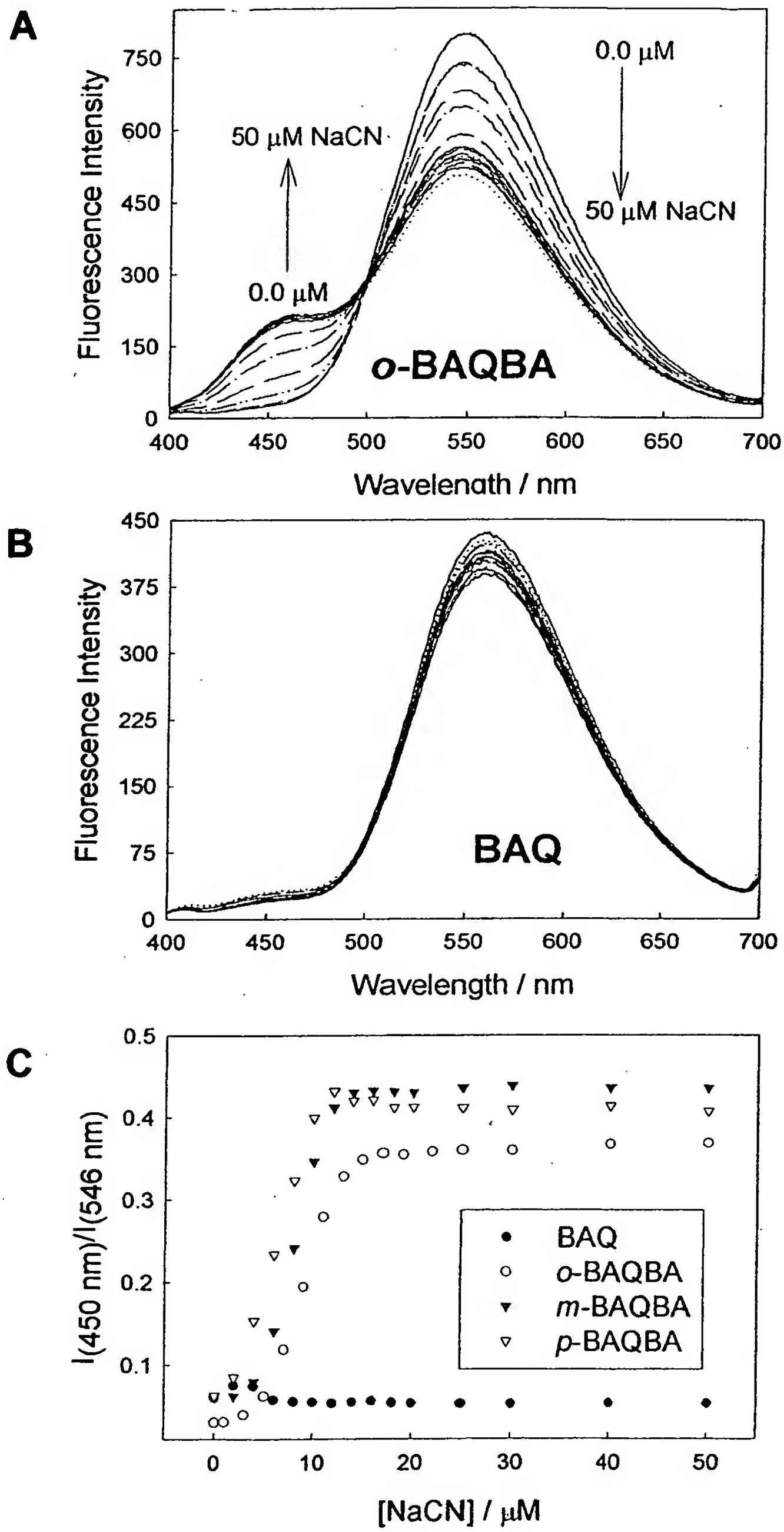

A
Fluorescence Intensity
750
600
450
300
150
0
50 μM NaCN
0.0 μM
0.0 μM
50 μM NaCN
o-BAQBA
400
450
500
550
600
650
700
Wavelength / nm
B
Fluorescence Intensity
450
375
300
225
150
75
0
BAQ
400
450
500
550
600
650
700
Wavelength / nm
C
I(450 nm)/I(546 nm)
0.5
0.4
0.3
0.2
0.1
BAQ
o-BAQBA
m-BAQBA
p-BAQBA
0
10
20
30
40
50
[NaCN] / μM

FIGURE 14

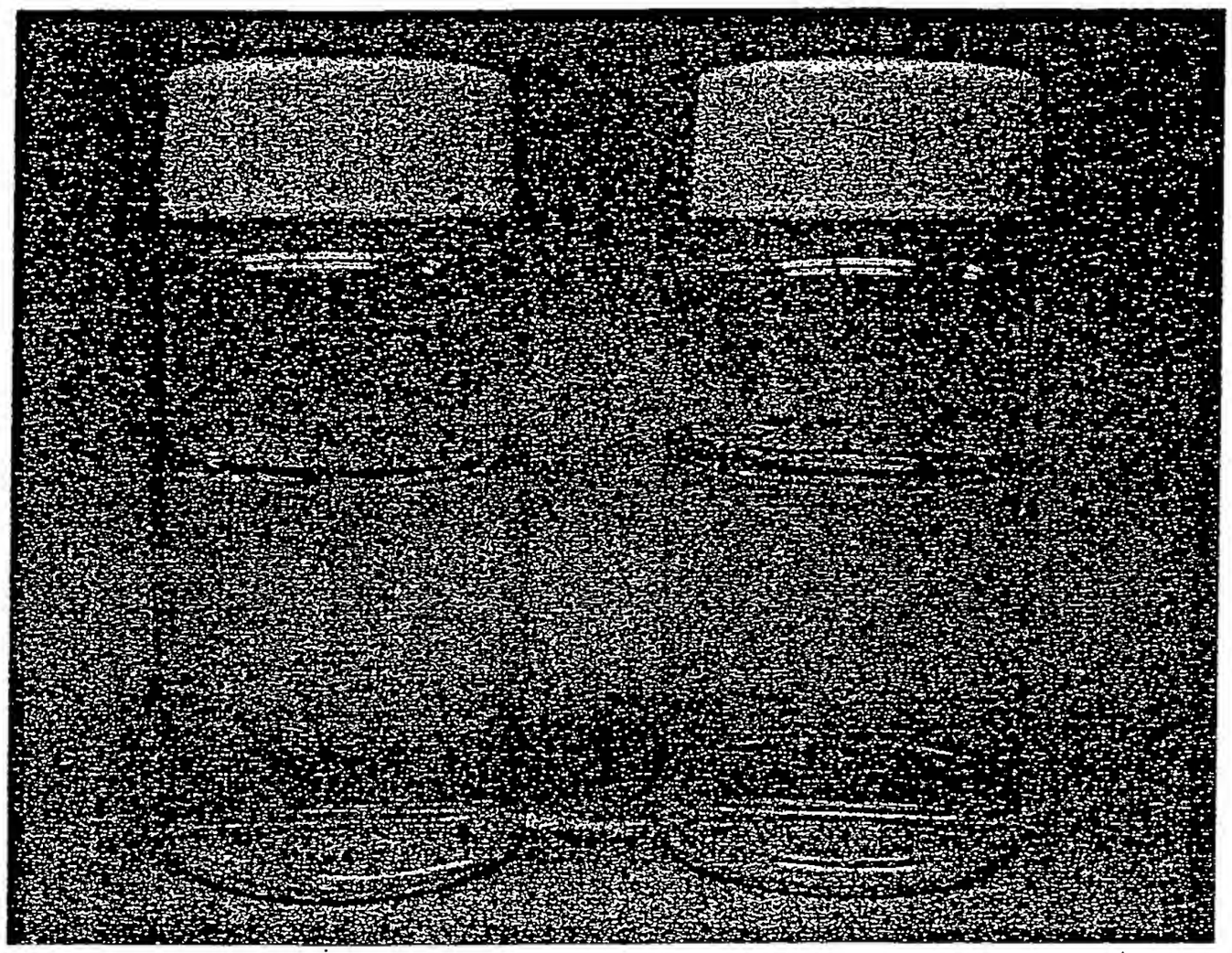
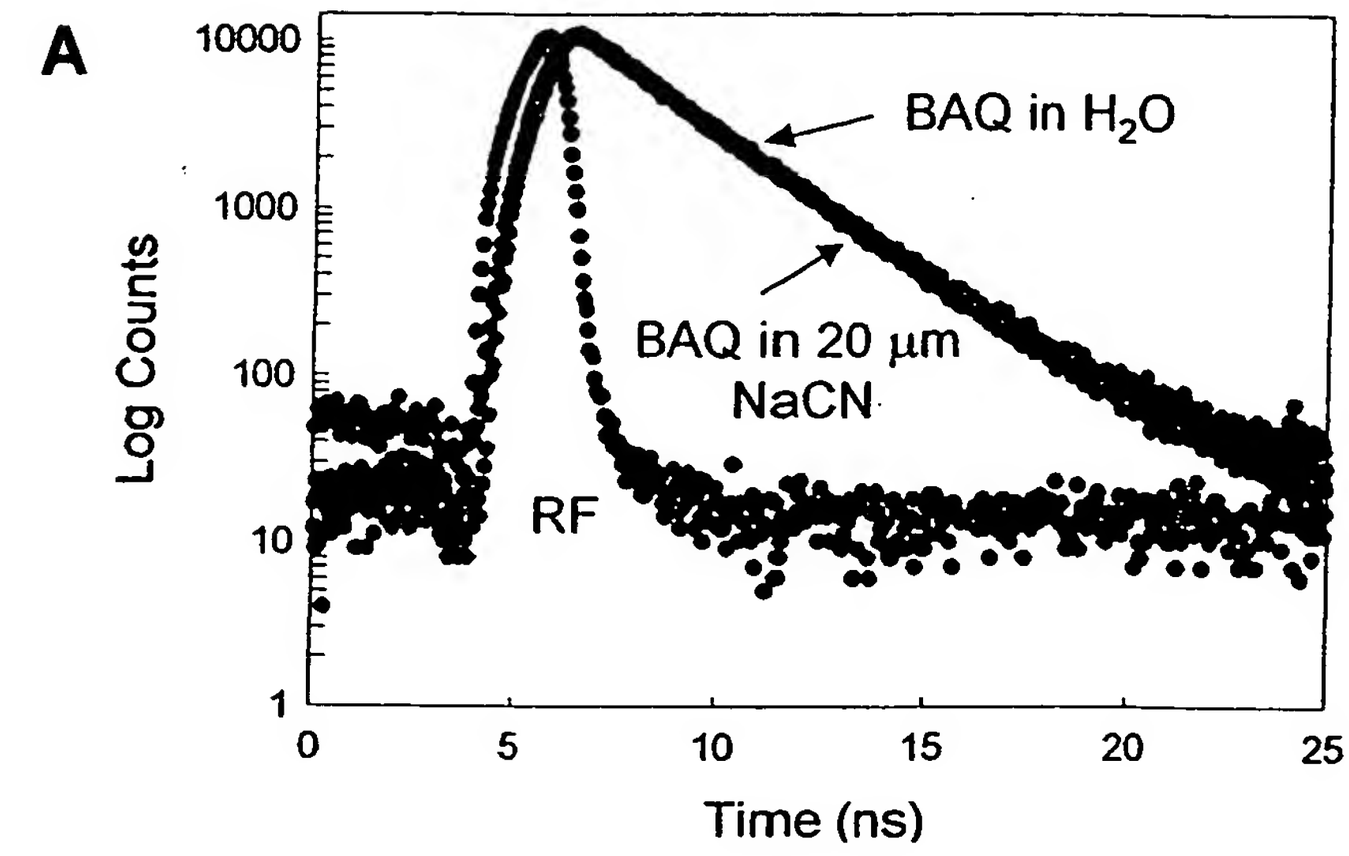


FIGURE 15


A
10000
1000
100
10
1
Log Counts
BAQ in H_2O
BAQ in 20 µm NaCN
RF
0
5
10
15
20
25
Time (ns)

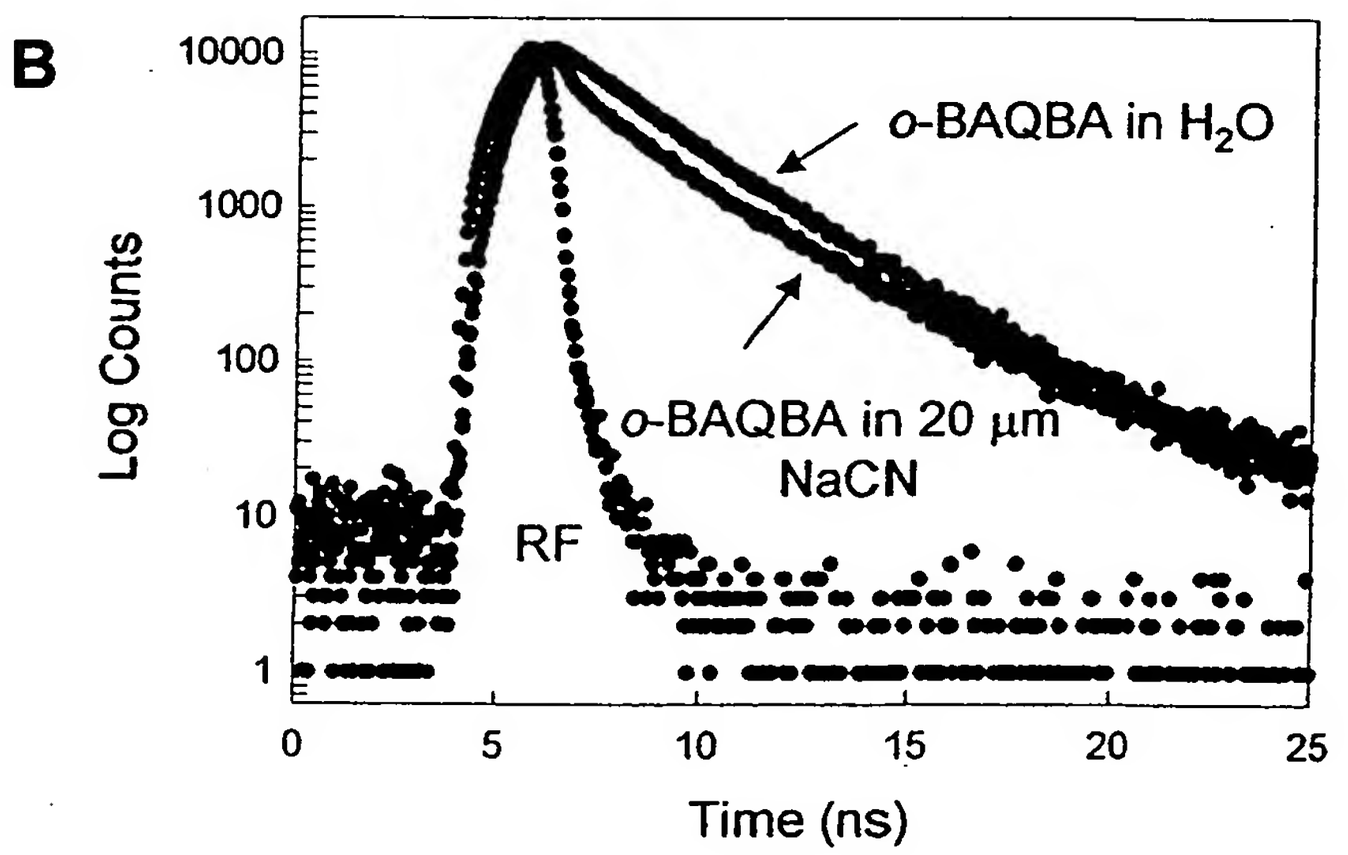

B
10000
1000
100
10
1
Log Counts
o-BAQBA in H_2O
o-BAQBA in 20 µm NaCN
RF
0
5
10
15
20
25
Time (ns)

FIGURE 16

Table 4: Multiexponential intensity decay of BAQ and *o*-BAQBA

[Cyanide] μM	τ_1 (ns)	α_1	τ_2 (ns)	α_2	τ_3 (ns)	α_3	$\bar{\tau}$	$\langle\tau\rangle$	χ^2
BAQ									
0	2.48	1	-	-	-	-	2.48	2.48	1.10
2	2.48	1	-	-	-	-	2.48	2.48	1.02
4	2.49	1	-	-	-	-	2.49	2.49	1.19
6	2.49	1	-	-	-	-	2.49	2.49	1.32
10	2.49	1	-	-	-	-	2.49	2.49	1.18
16	2.49	1	-	-	-	-	2.49	2.49	1.28
20	2.47	1	-	-	-	-	2.47	2.47	0.89
***o*-BAQBA**									
(380 nm)[a]									
0	2.04	0.71	3.41	0.29	-	-	2.59	2.44	1.06
2	2.02	0.68	3.367	0.32	-	-	2.61	2.45	0.99
4	1.98	0.67	3.37	0.33	-	-	2.61	2.44	0.94
6	1.92	0.62	3.23	0.38	-	-	2.59	2.42	1.06
8[c]	1.55	0.41	2.98	0.59	-	-	2.60	2.39	1.53
10[c]	0.67	0.19	2.64	0.81	-	-	2.53	2.27	2.15
12.5	0.44	0.22	2.60	0.78	-	-	2.50	2.12	2.37
	0.21	0.17	2.07	0.63	3.99	0.20	2.76	2.14	1.08
15	0.38	0.28	2.61	0.72	-	-	2.49	1.98	2.18
	0.21	0.23	1.85	0.44	3.46	0.32	2.71	1.97	1.01
20	0.38	0.30	2.65	0.70	-	-	2.52	1.97	2.47
	0.19	0.24	1.69	0.39	3.36	0.37	2.72	1.95	1.12
(550 nm)[b]									
0	1.99	0.63	3.19	0.37	-	-	2.57	2.43	0.99
2	1.93	0.59	3.15	0.41	-	-	2.58	2.43	0.98
4	2.04	0.70	3.39	0.30	-	-	2.60	2.45	1.07
6	1.87	0.51	2.97	0.49	-	-	2.53	2.41	1.10
8	1.86	0.55	3.14	0.45	-	-	2.60	2.44	1.01
10	1.75	0.48	3.10	0.52	-	-	2.63	2.45	1.17
12.5	1.85	0.61	3.48	0.39	-	-	2.74	2.49	1.03
15	1.32	0.31	2.93	0.69	-	-	2.66	2.43	1.25
20	1.19	0.30	2.97	0.70	-	-	2.71	2.44	0.92

[a]380 nm long-pass filter.
[b]550±10 nm interference filter.
[c]No notable improvement in fit could be obtained using a 3-exponent function. Similar values were also found for the *meta*- and *para*-BAQBA probes.

FIGURE 17

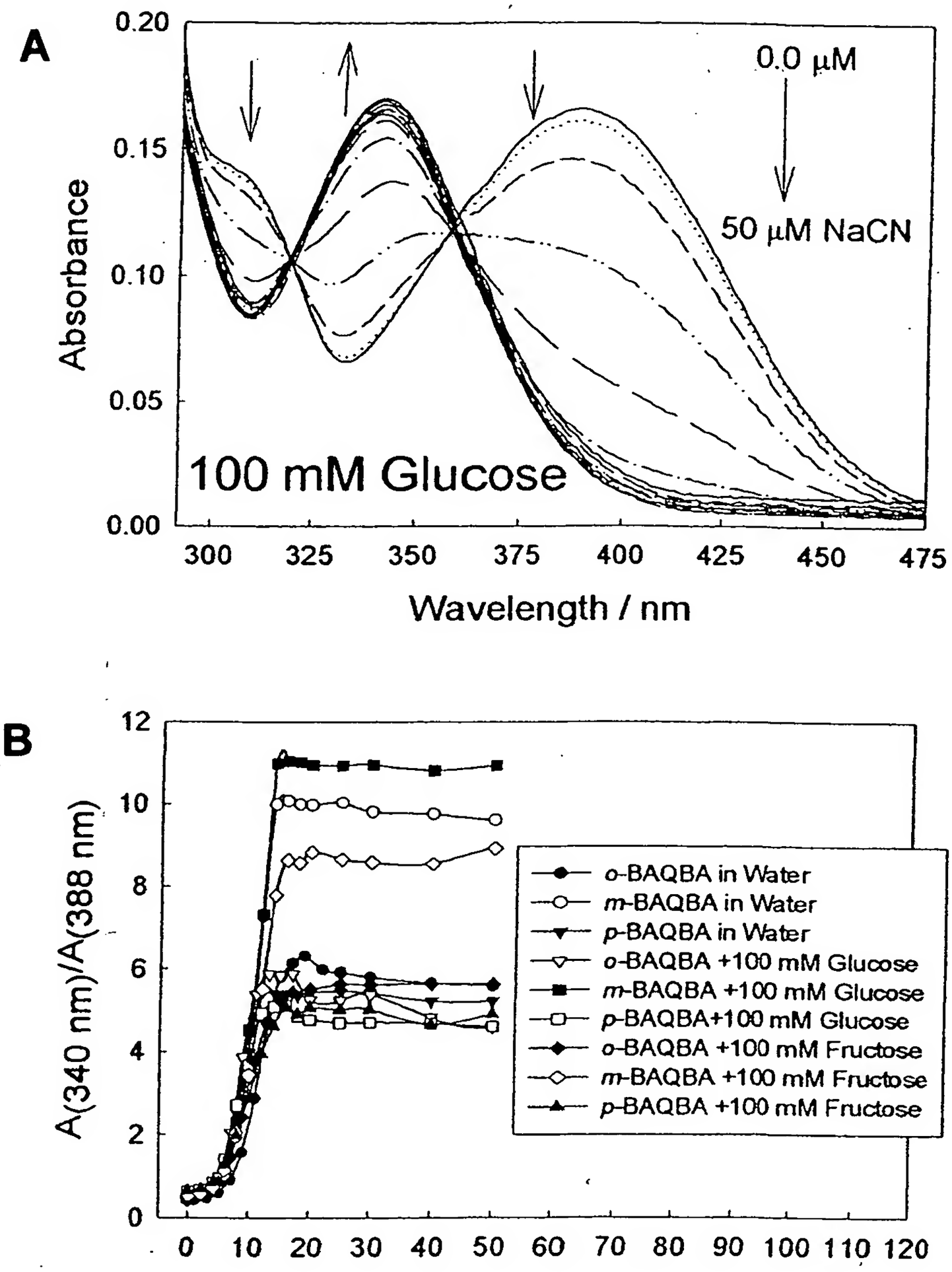
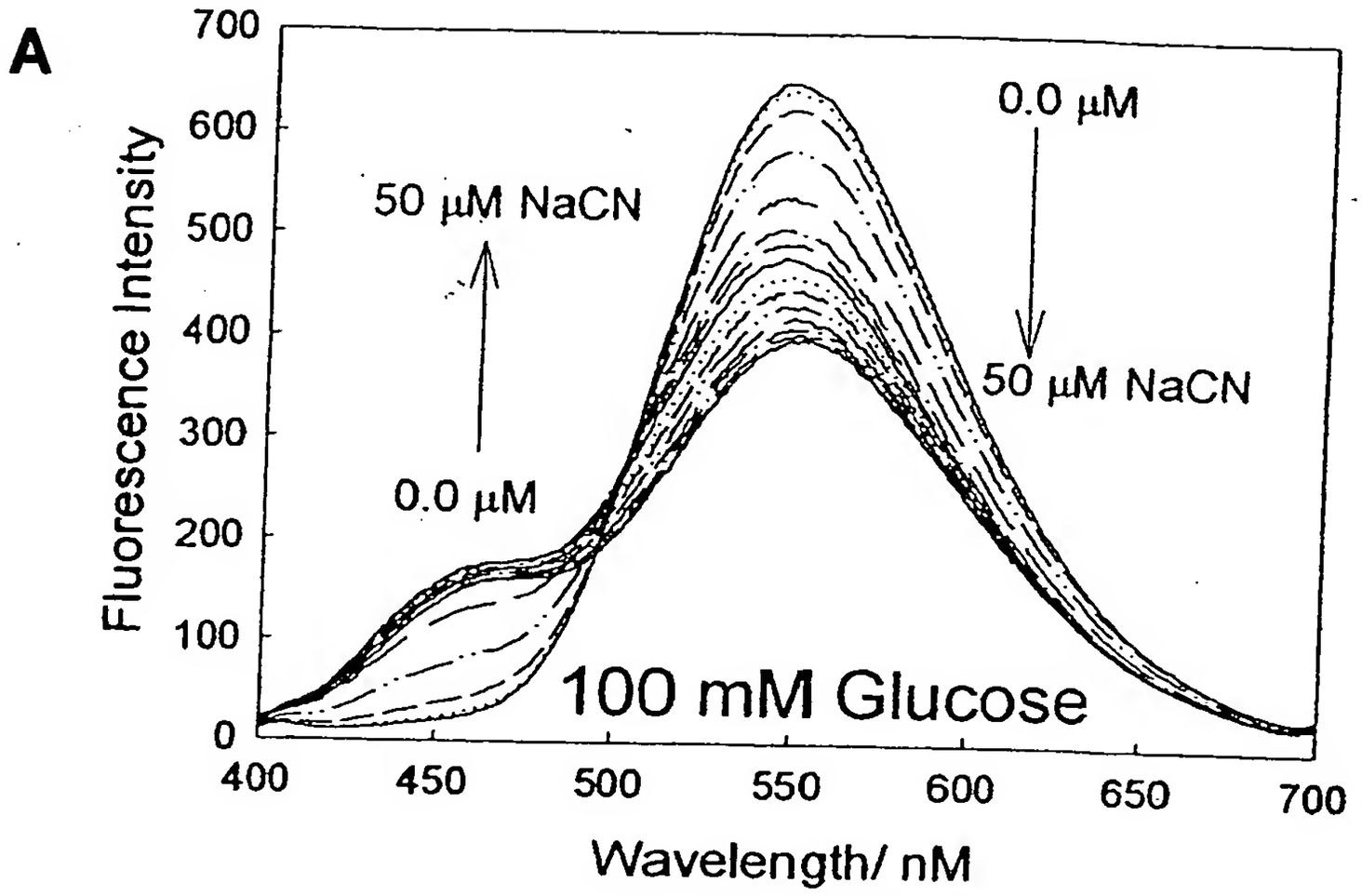

A
0.20
0.15
0.10
0.05
0.00
Absorbance
0.0 µM
50 µM NaCN
100 mM Glucose
300
325
350
375
400
425
450
475
Wavelength / nm
B
12
10
8
6
4
2
0
A(340 nm)/A(388 nm)
o-BAQBA in Water
m-BAQBA in Water
p-BAQBA in Water
o-BAQBA +100 mM Glucose
m-BAQBA +100 mM Glucose
p-BAQBA+100 mM Glucose
o-BAQBA +100 mM Fructose
m-BAQBA +100 mM Fructose
p-BAQBA +100 mM Fructose
0
10
20
30
40
50
60
70
80
90
100
110
120
[NaCN] / µM

FIGURE 18


A
Fluorescence Intensity
700
600
500
400
300
200
100
0
400
450
500
550
600
650
700
Wavelength/ nM
50 μM NaCN
0.0 μM
0.0 μM
50 μM NaCN
100 mM Glucose

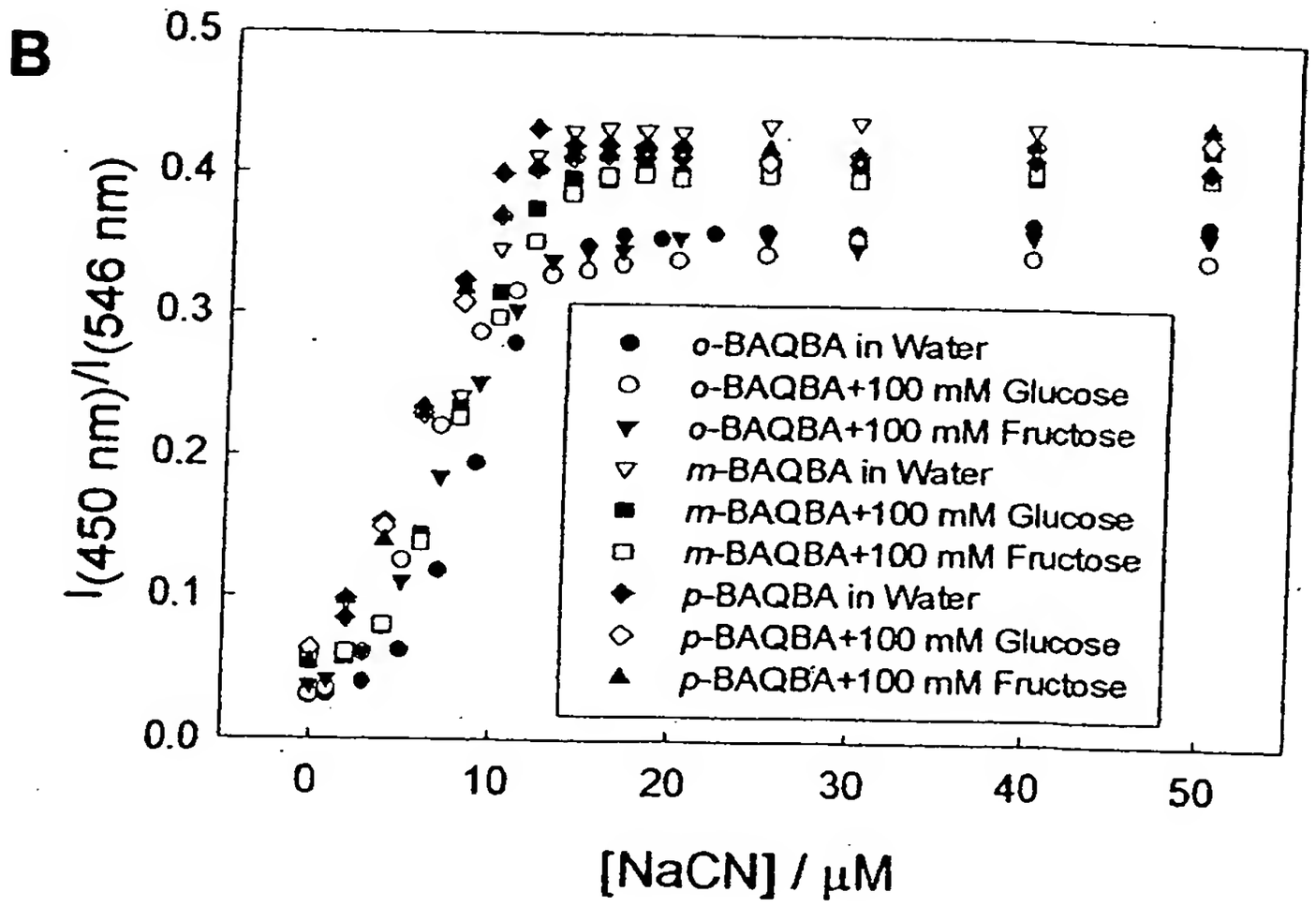
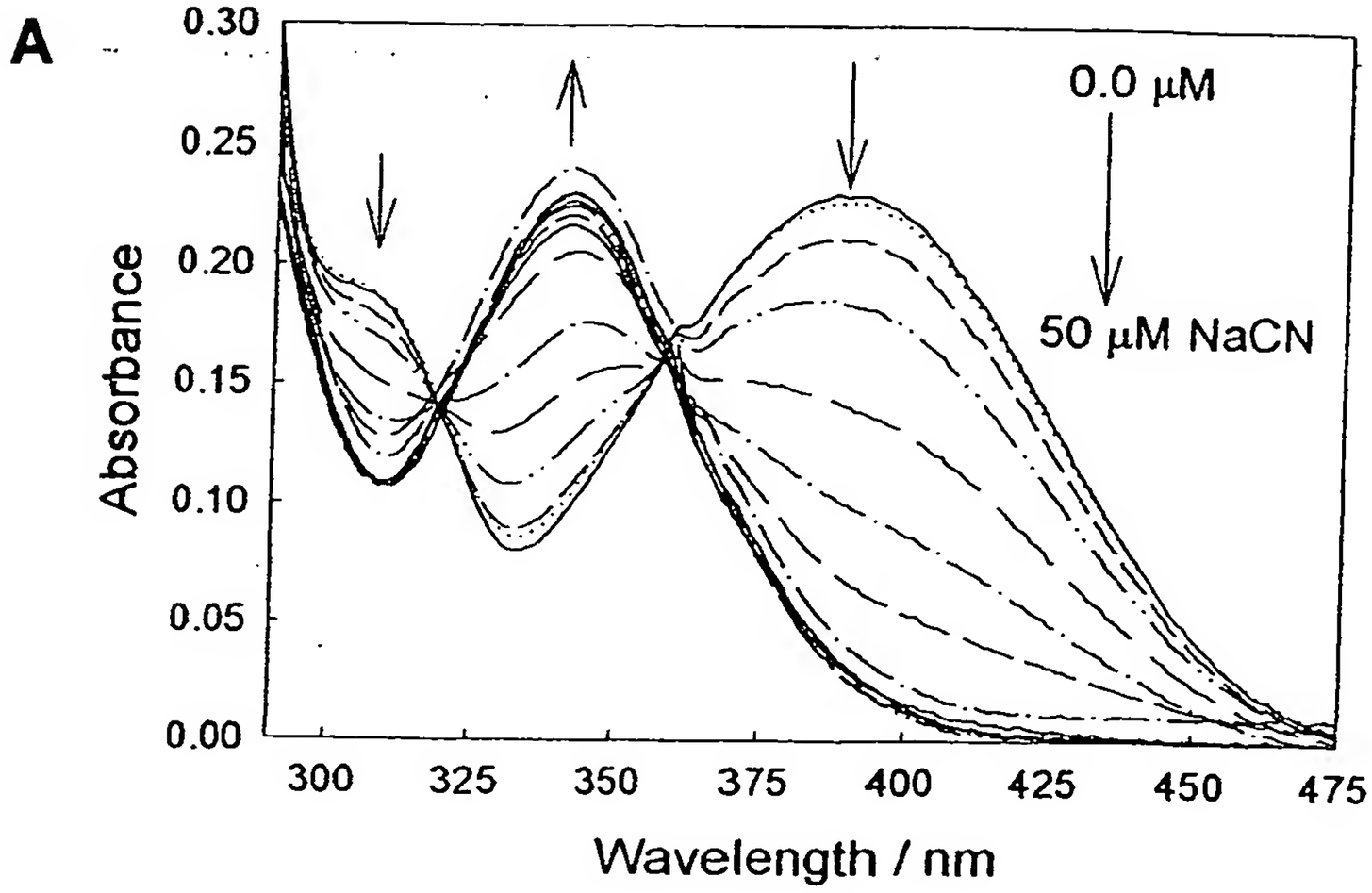

B
I(450 nm)/I(546 nm)
0.5
0.4
0.3
0.2
0.1
0.0
0
10
20
30
40
50
[NaCN] / μM
o-BAQBA in Water
o-BAQBA+100 mM Glucose
o-BAQBA+100 mM Fructose
m-BAQBA in Water
m-BAQBA+100 mM Glucose
m-BAQBA+100 mM Fructose
p-BAQBA in Water
p-BAQBA+100 mM Glucose
p-BAQBA+100 mM Fructose

FIGURE 19


A
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Absorbance
0.0 μM
50 μM NaCN
300
325
350
375
400
425
450
475
Wavelength / nm

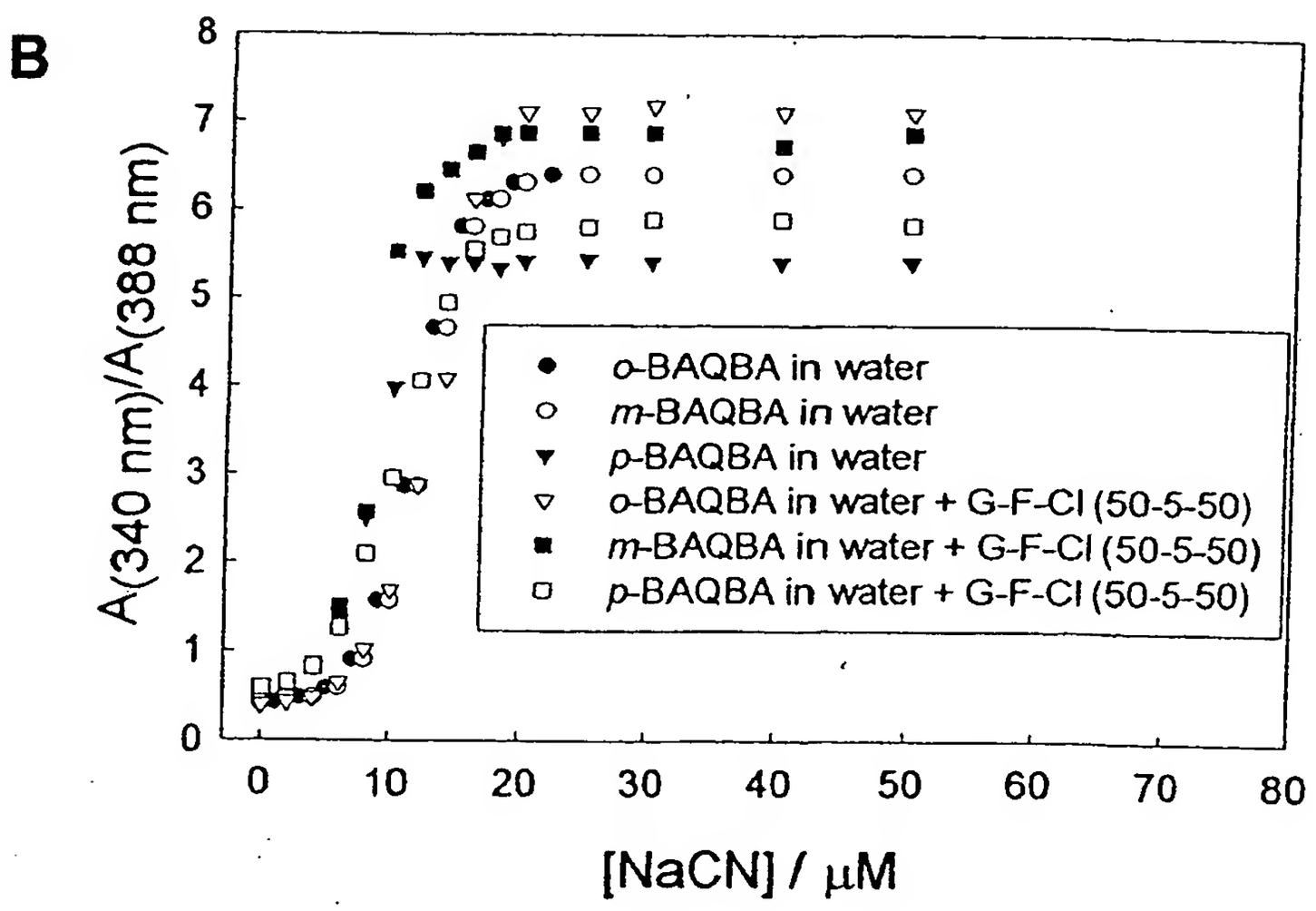
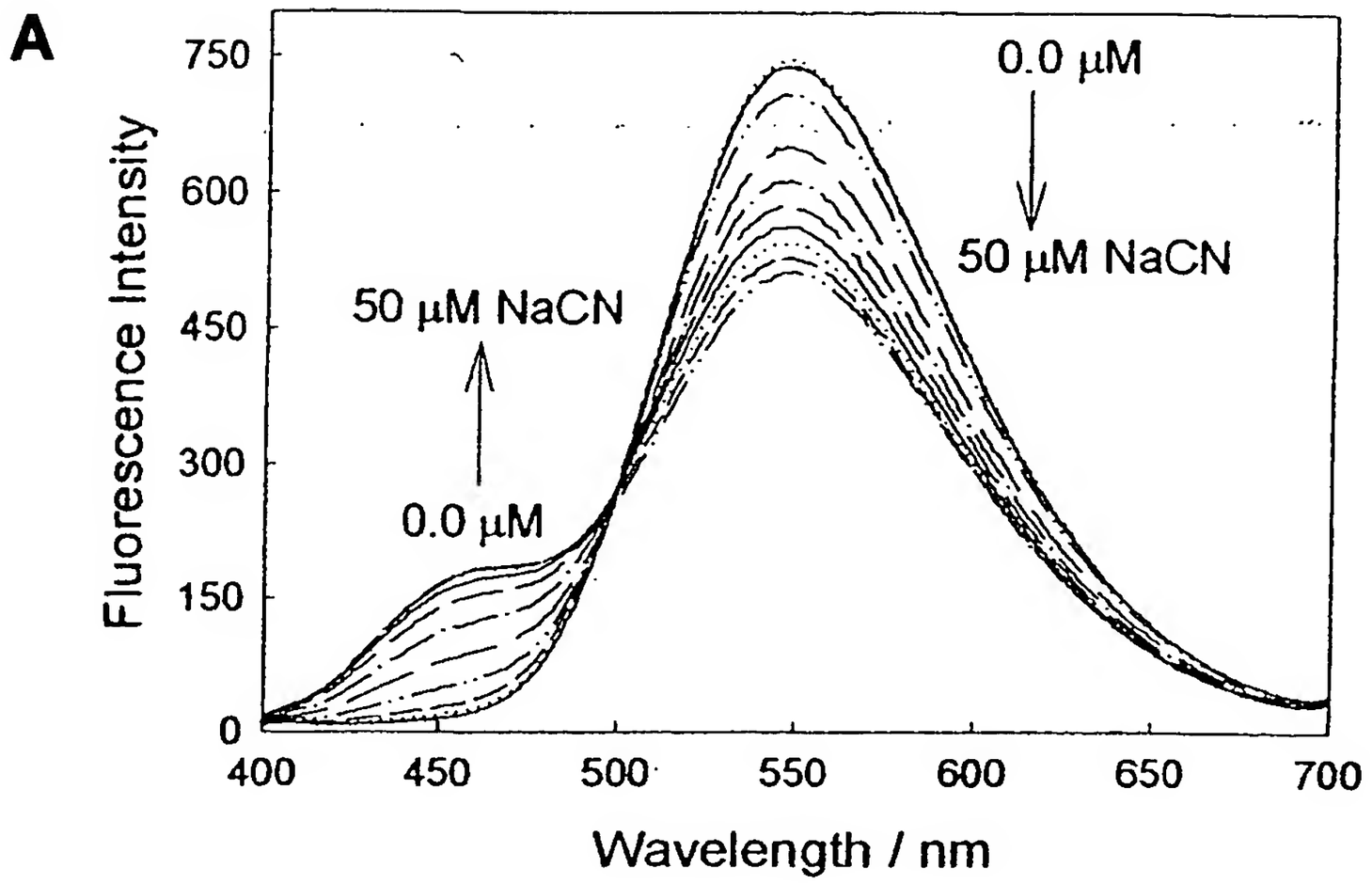

B
8
7
6
5
4
3
2
1
0
A(340 nm)/A(388 nm)
o-BAQBA in water
m-BAQBA in water
p-BAQBA in water
o-BAQBA in water + G-F-Cl (50-5-50)
m-BAQBA in water + G-F-Cl (50-5-50)
p-BAQBA in water + G-F-Cl (50-5-50)
0
10
20
30
40
50
60
70
80
[NaCN] / μM

FIGURE 20


A
750
600
450
300
150
0
Fluorescence Intensity
0.0 μM
50 μM NaCN
50 μM NaCN
0.0 μM
400
450
500
550
600
650
700
Wavelength / nm

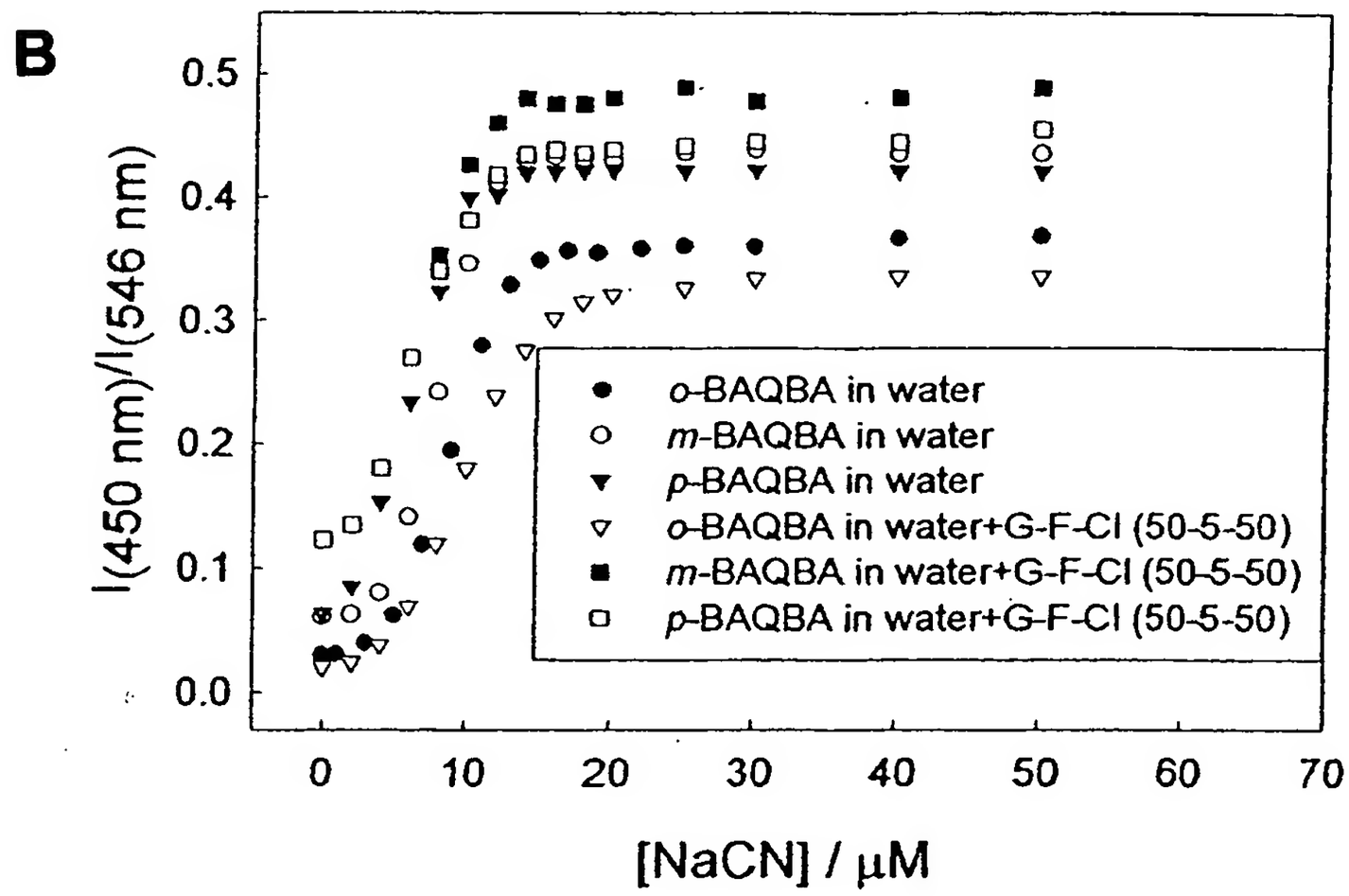
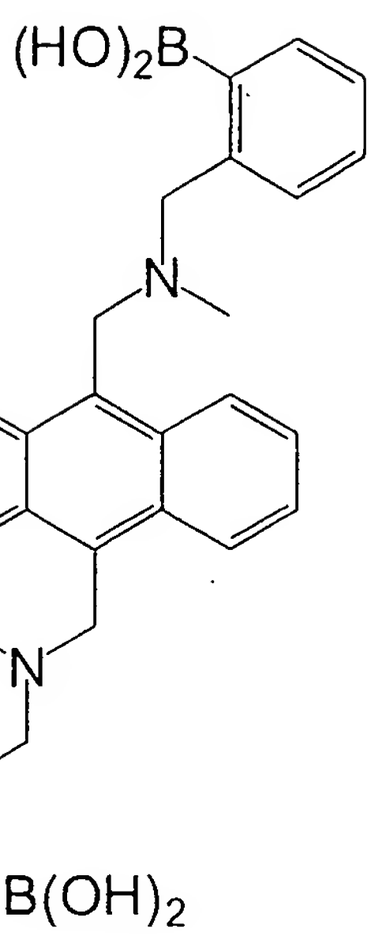
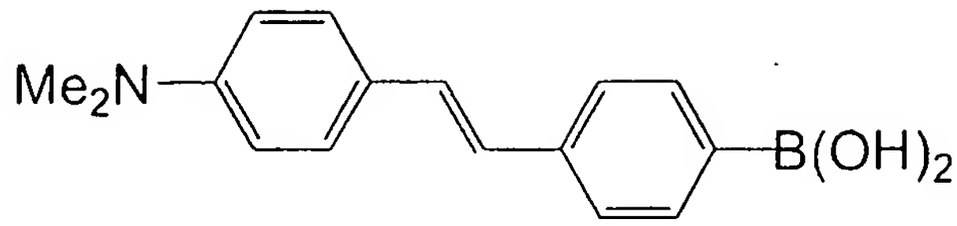

B
0.5
0.4
0.3
0.2
0.1
0.0
I(450 nm)/I(546 nm)
o-BAQBA in water
m-BAQBA in water
p-BAQBA in water
o-BAQBA in water+G-F-Cl (50-5-50)
m-BAQBA in water+G-F-Cl (50-5-50)
p-BAQBA in water+G-F-Cl (50-5-50)
0
10
20
30
40
50
60
70
[NaCN] / μM

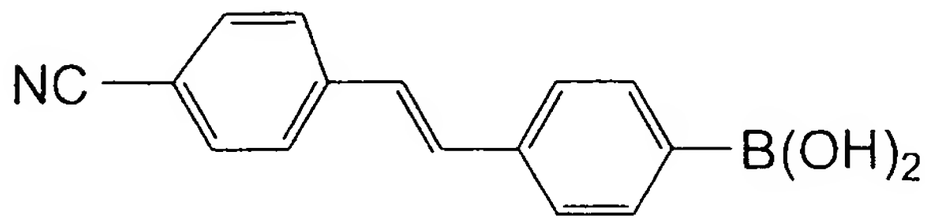
FIGURE 21



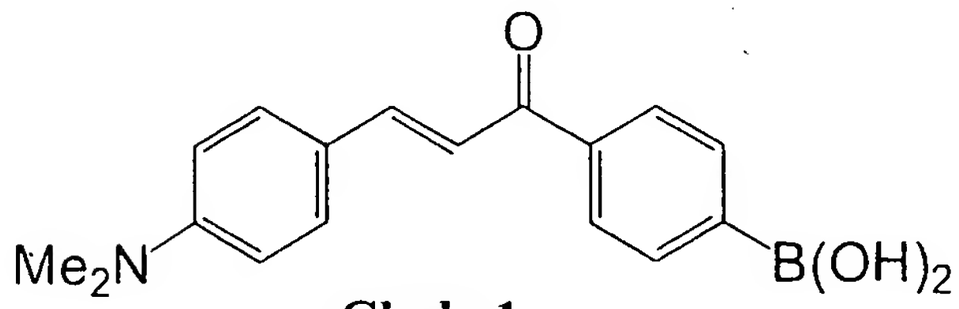
ANDBA



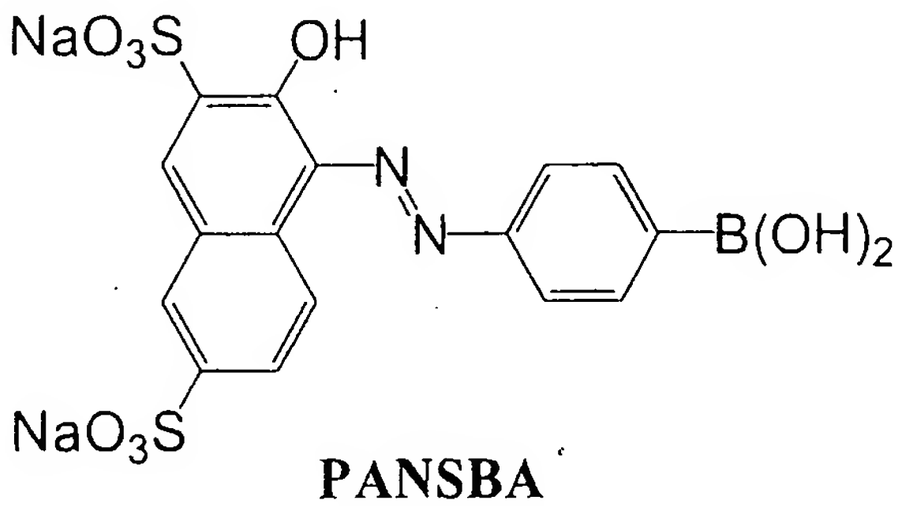
DSTBA



CSTBA

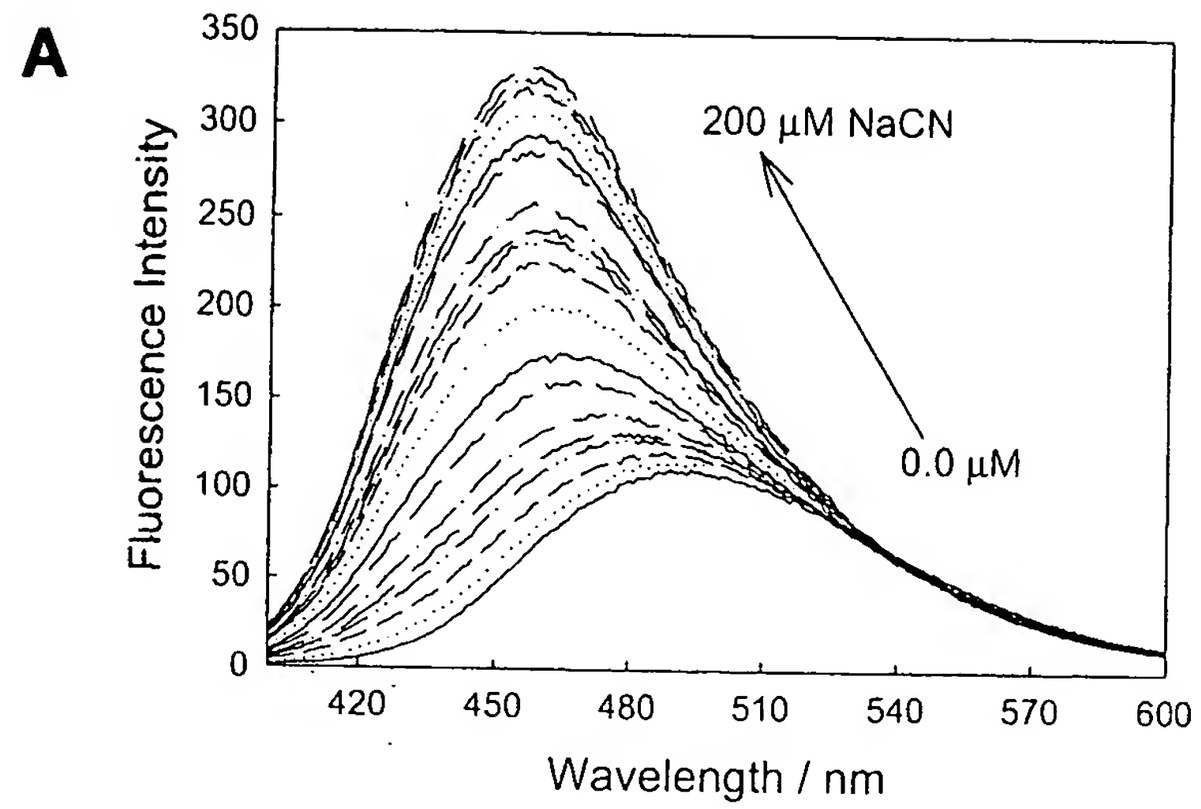


Chalc 1



PANSBA

FIGURE 22


A
Fluorescence Intensity
350
300
250
200
150
100
50
0
200 µM NaCN
0.0 µM
420
450
480
510
540
570
600
Wavelength / nm

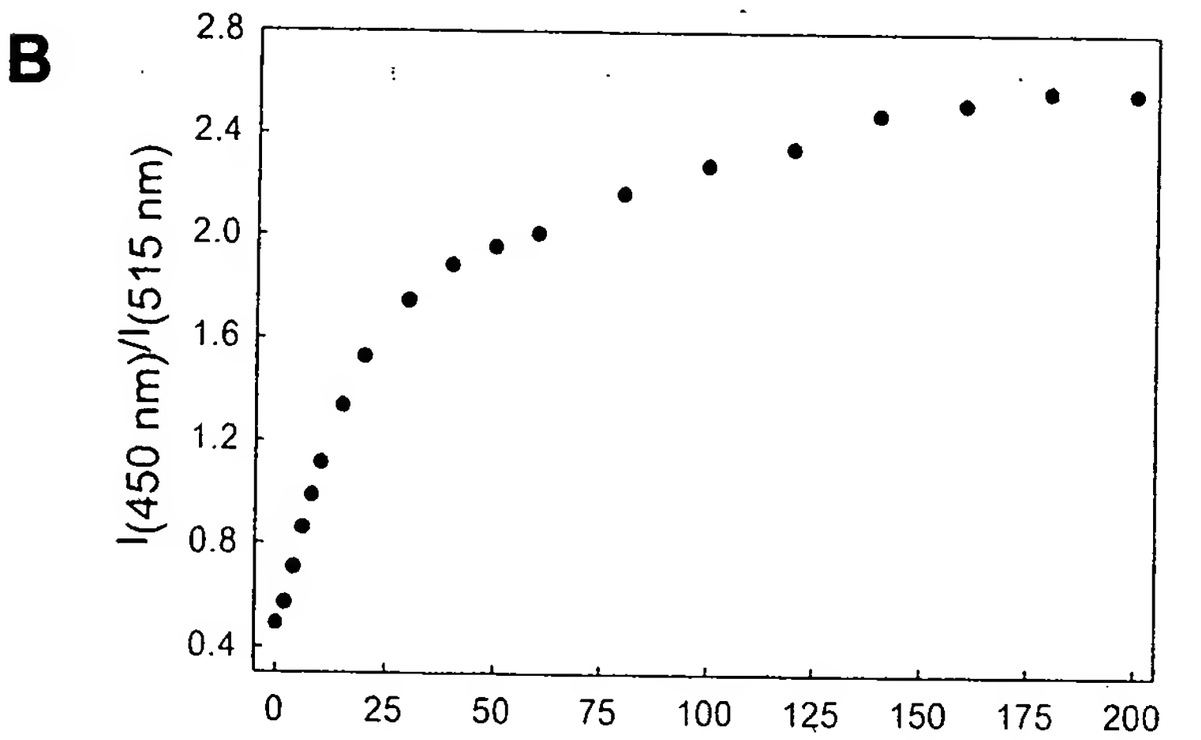
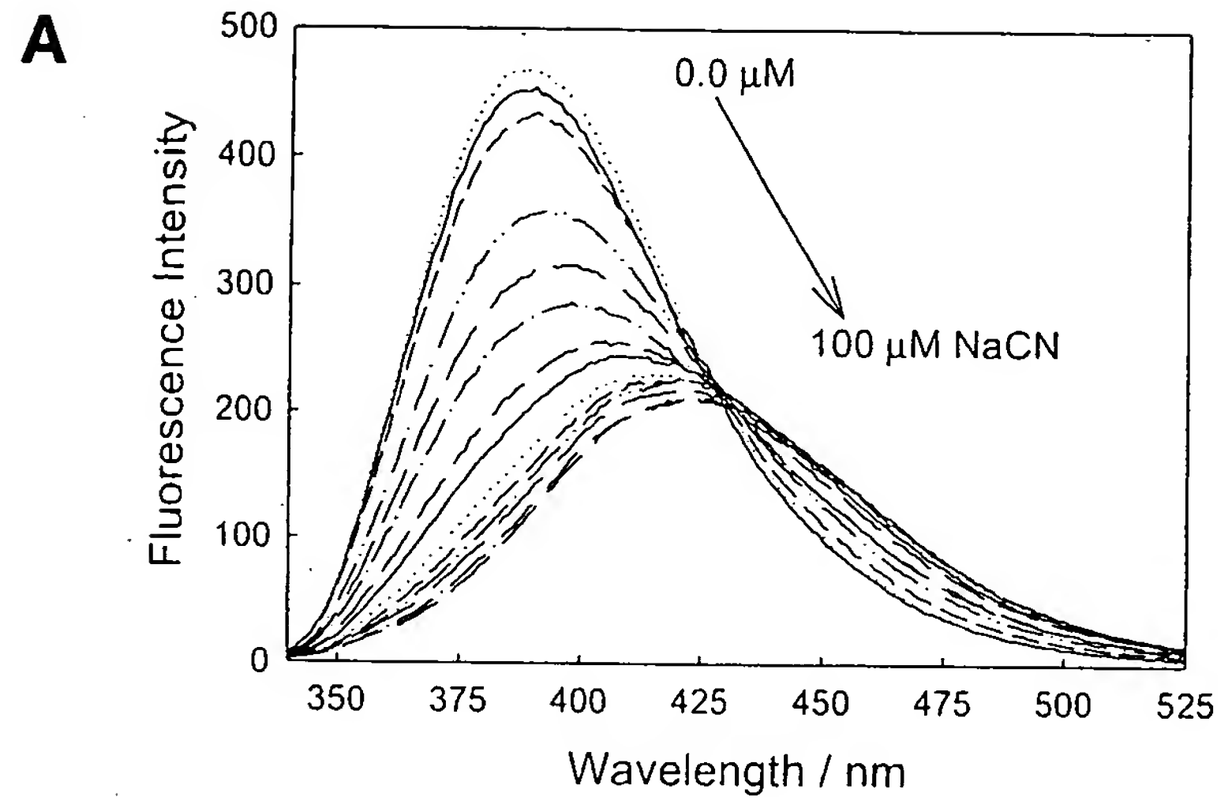

B
I(450 nm)/I(515 nm)
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0
25
50
75
100
125
150
175
200
[NaCN] / µM

FIGURE 23


A
500
400
300
200
100
0
Fluorescence Intensity
0.0 µM
100 µM NaCN
350
375
400
425
450
475
500
525
Wavelength / nm

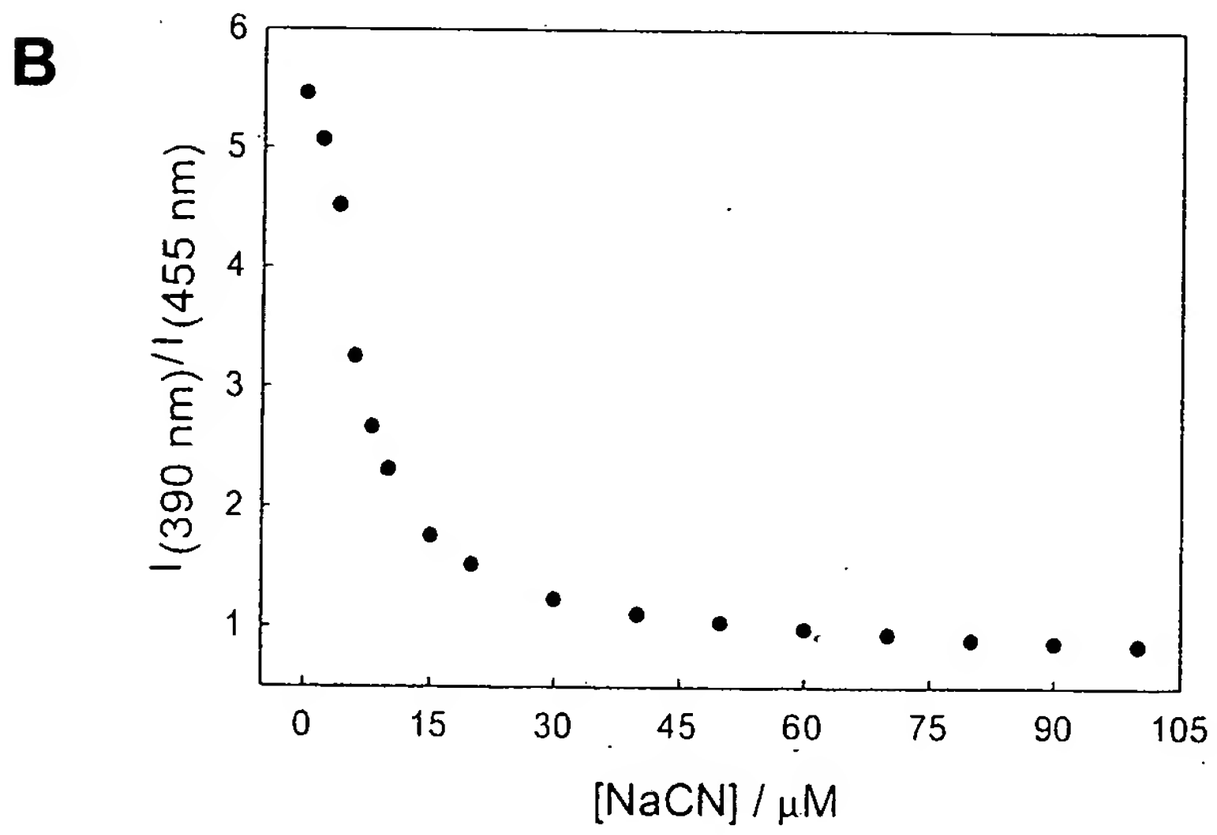

B
6
5
4
3
2
1
I(390 nm)/I(455 nm)
0
15
30
45
60
75
90
105
[NaCN] / µM

FIGURE 24

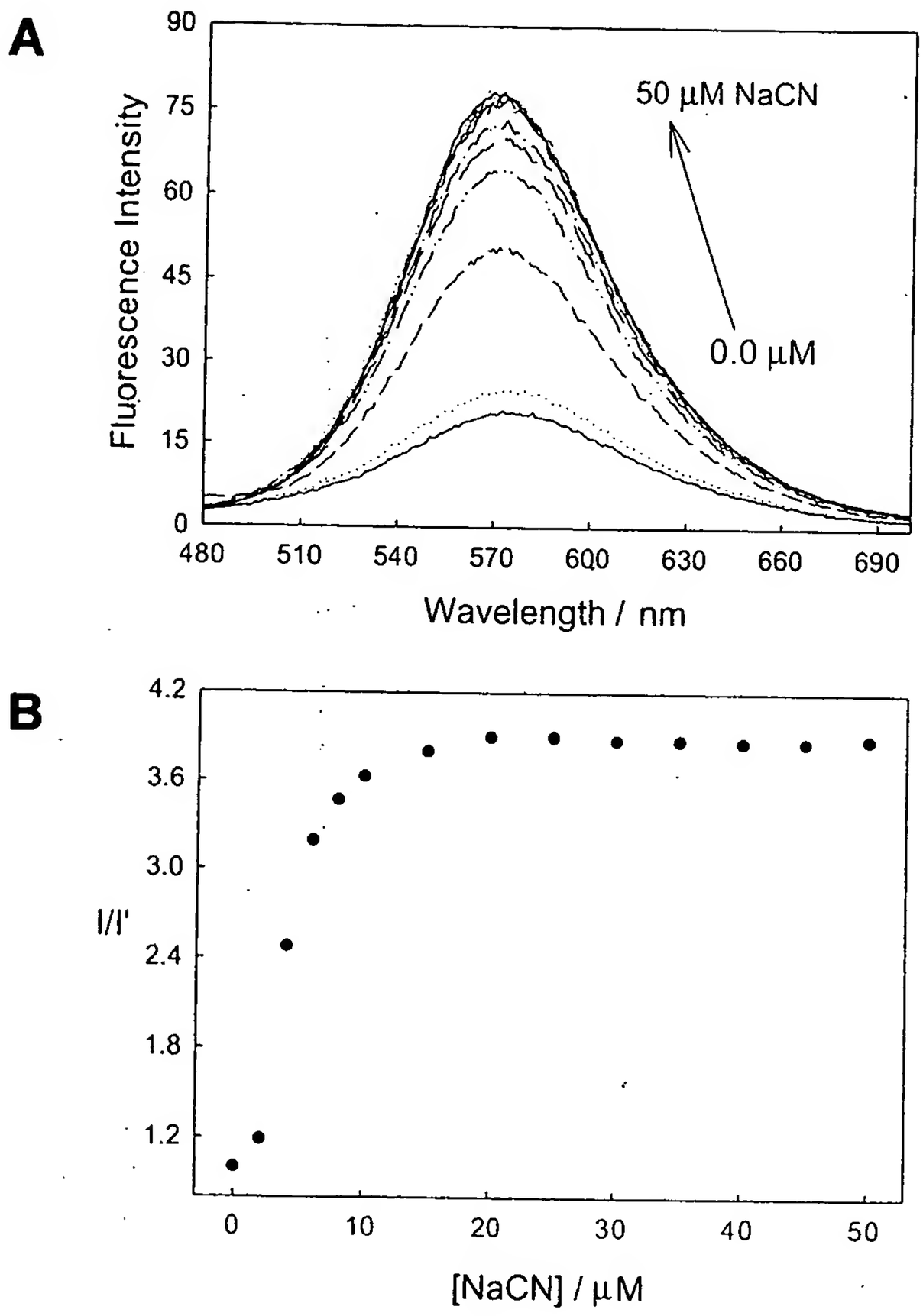
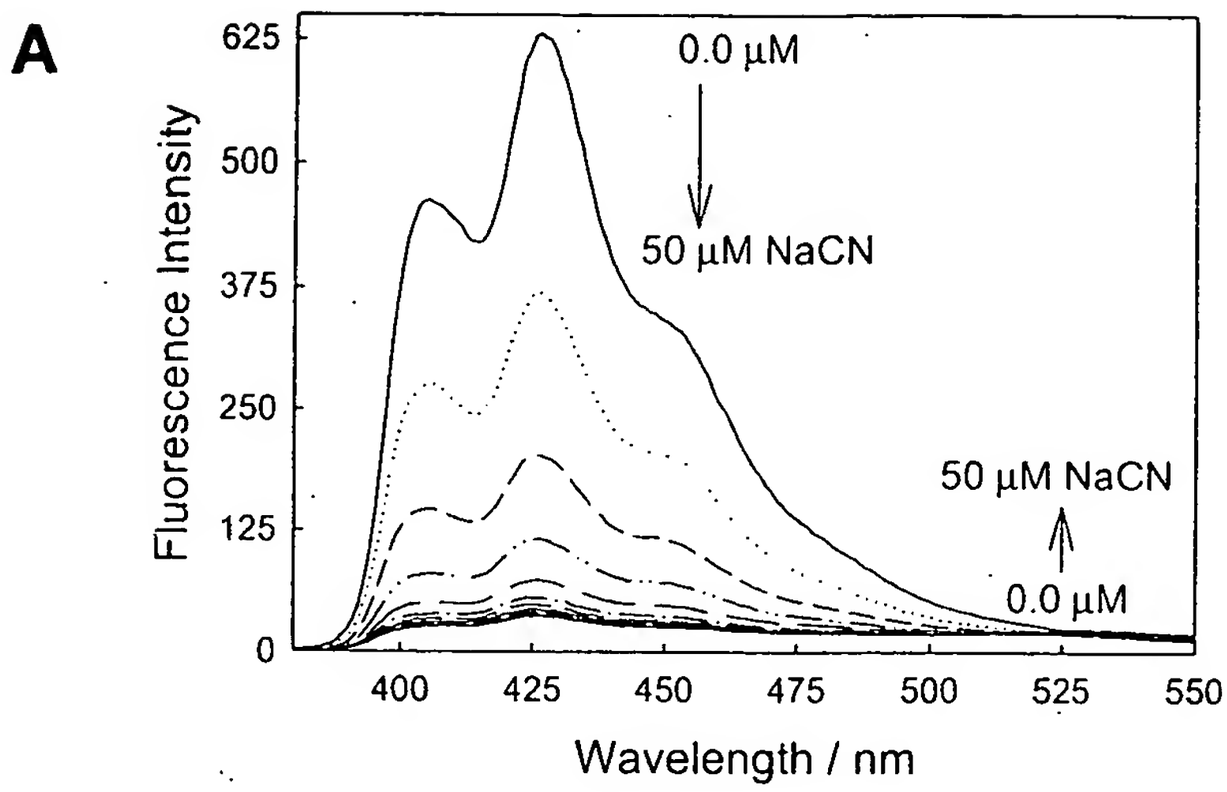

A
Fluorescence Intensity
Wavelength / nm
50 µM NaCN
0.0 µM
B
I/I'
[NaCN] / µM

FIGURE 25


A
625
500
375
250
125
0
Fluorescence Intensity
0.0 µM
50 µM NaCN
50 µM NaCN
0.0 µM
400
425
450
475
500
525
550
Wavelength / nm

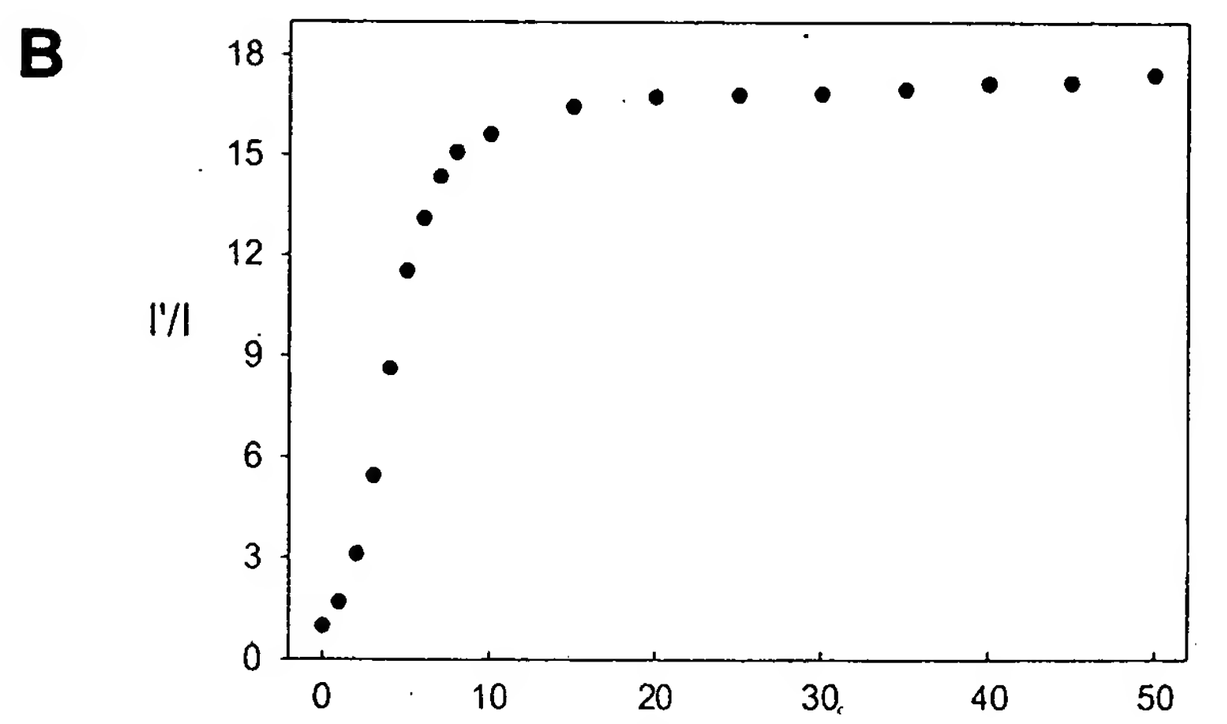

B
18
15
12
9
6
3
0
I'/I
0
10
20
30
40
50
[NaCN] / µM

FIGURE 26

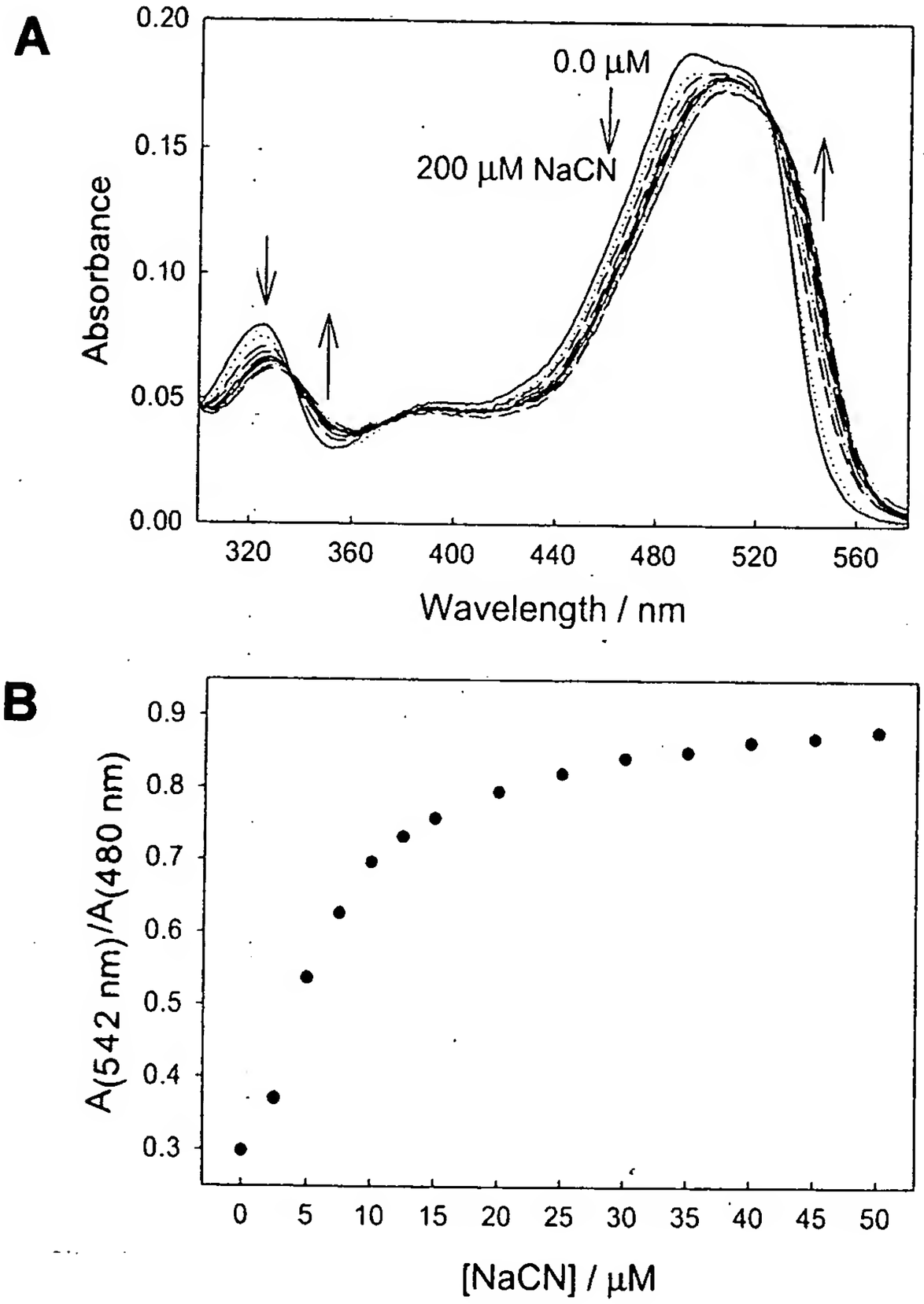

A
0.20
0.15
0.10
0.05
0.00
Absorbance
0.0 µM
200 µM NaCN
320
360
400
440
480
520
560
Wavelength / nm
B
0.9
0.8
0.7
0.6
0.5
0.4
0.3
A(542 nm)/A(480 nm)
0
5
10
15
20
25
30
35
40
45
50
[NaCN] / µM

FIGURE 27

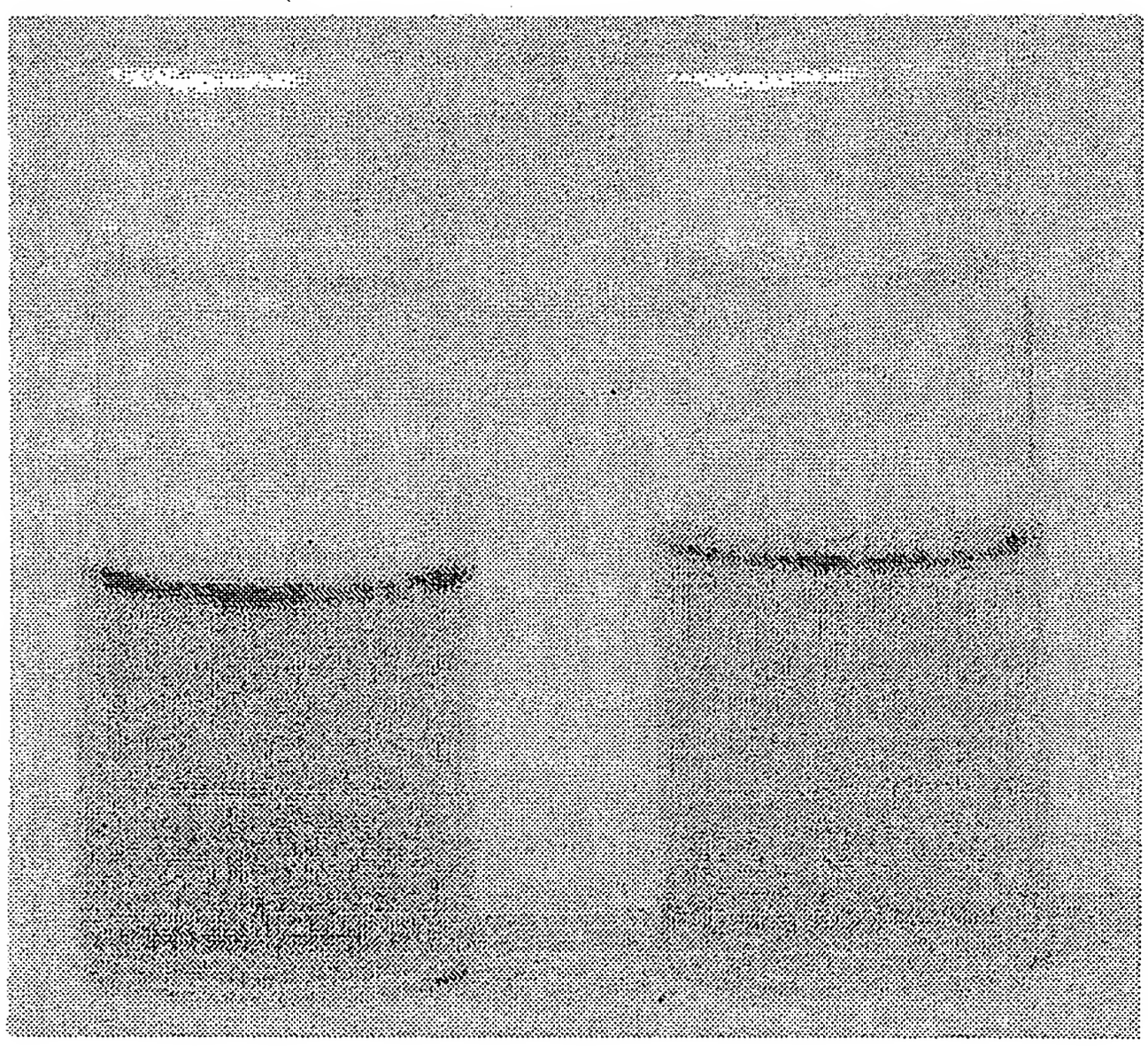


FIGURE 28